THE UNIVERSITY OF ALBERTA

BINARY DISTILLATION COLUMN CONTROL:
EFFECT OF SENSOR LOCATION

BY

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A THESIS

SUBMITTED TO THE FACULTY OF GRADUATE STUDIES

IN PARTIAL FULFILMENT OF THE REQUIREMENTS FOR THE DEGREE

OF MASTER OF SCIENCE

DEPARTMENT OF CHEMICAL AND PETROLEUM ENGINEERING

EDMONTON, ALBERTA

FALL, 1971

UNIVERSITY OF ALBERTA

FACULTY OF GRADUATE STUDIES

The undersigned certify that they have read, and recommend to the Faculty of Graduate Studies for acceptance a thesis entitled BINARY DISTILLATION COLUMN CONTROL: EFFECT OF SENSOR LOCATION submitted by Bui Minh Chanh in partial fulfilment of the requirements for the degree of Master of Science in Chemical Engineering.

ABSTRACT

This thesis investigates the effect of the sensor location on the control performance of binary distillation columns with no side-stream drawoffs.

The performance of two pilot-scale distillation columns has been investigated by digital simulation: a two-feet diameter, ten-tray bubble cap column separating an acetone-benzene system located at the University of Delaware and the nine-inch diameter, eight-tray bubble cap column separating a methanol-water mixture installed at the University of Alberta.

The dynamics of both columns were represented by means of transfer functions based on experimental data from pulse testing or the step responses of the columns. Several procedures were used for obtaining approximate transfer functions; the Rosenbrock optimizing program has been used to fit the time-domain data and the methods of Bailey and Law, Chen and Philip, Levy, Staffin and Staffin and Rosenbrock have been employed to fit the frequency-domain data. As time-domain data are more readily available, the Rosenbrock method has been utilized whenever possible to determine the distillation process transfer functions. It was found that the dynamics of the column as predicted from the models showed satisfactory agreement with experimental data especially when the magnitudes of perturbations were not large.

Feedback control and combined feedforward-feedback control of

top product composition, of bottom product composition and of the liquid temperature (or composition) on an intermediate tray using reflux or steam as the manipulative variable have been investigated by simulation. For the University of Delaware column, a stepwise variation of 5 mole per cent of acetone was used as the forcing function, whereas for the University of Alberta column, a step change in feed flow rate from 50 per cent to 70 per cent on the feed flow recording chart was used as the forcing function.

Simulation results revealed that top product composition was best controlled by manipulation of reflux flow with direct sensing of overhead composition preferred. If by necessity, measurement at an intermediate tray is required, the sensor should be located as close to the top tray as possible. Bottom product composition was best controlled by manipulation of steam flow. Whenever steam is used as the corrective medium, generally, the sensor should be situated where if the liquid temperature (or composition) on this tray is maintained constant, it would result in the least offset in product purity.

Feedback control of the liquid temperature on an intermediate tray has been evaluated experimentally using the University of Alberta column. Since all experimental tests were conducted for disturbances in feed flow rate of large magnitudes, the simulation results did not predict very satisfactorily the steady-state errors observed experimentally. Despite the lack of precise agreement, the models used in the simulation study proved very helpful in comparing the performance of the column for different locations of the sensing element.

ACKNOWLEDGMENTS

The author is greatly indebted to his thesis supervisor, Dr. R.K. Wood for his most helpful advices, suggestions and comments.

Grateful acknowledgment is due to the University of Alberta Computing Centre and the Data Acquisition, Control and Simulation Centre in the Department of Chemical and Petroleum Engineering for the ample use of their computing facilities.

Deep and sincere appreciation is made to all those who have contributed in various ways to the preparation of the manuscript.

The author was supported at times by the Canadian International Development Agency and the Department of Chemical and Petroleum Engineering.

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CHAPTER I

INTRODUCTION

The primary object of control of a distillation column will be to keep at least one product within specification despite external disturbances which may enter the system such as feed flow rate, feed composition, etc. The present investigation will be limited to a binary distillation column which has only a single feed stream and no intermediate product streams.

Automatic control of product quality is usually accomplished in one of two ways:

(i) Holding a constant rate of heat input and varying the reflux rate to the top of the column so that the resulting material balance yields the desired overhead product.

(ii) Fixing the reflux at a constant rate and adjusting the heat input into the bottom of the column to yield a desired bottom product.

In order to achieve the control of a distillation column, it will usually be necessary to make at least one measurement of composition. However, despite the great advances in on-line analysis techniques in recent years, it is not always feasible to measure composition with sufficient speed and accuracy to provide the necessary information for the control system. A common indirect method of gauging product quality is the measurement of the temperature of the liquid at its boiling point.

Indeed, at equilibrium conditions, for a binary system under constant pressure and for a given temperature, the composition is completely specified.

At first glance, it might appear advantageous to control either the overhead or the bottom product composition simply by locating the sensor in the overhead or the bottom product line however, rarely is this the case. This is because in order for a controller to operate, the variable which it is controlling must be permitted to vary some, because a controller can only produce a change in valve position consequent upon a change in the controlled variable. As the system is designed so that the compositions (or temperatures) at both ends of the column are insensitive to disturbances, a composition (or temperature) measurement several plates removed from the ends of the column will provide more sensitive control. Also, at the ends of the column, the effects of pressure variations on the temperature of the liquid at its boiling point can swamp the effects of composition changes. However, as the control tray is moved farther away from the product to be controlled, the steady-state error increases and there is deterioration in the dynamic performance of the column. Therefore, in selecting the best control tray, a trade-off must be made between the control performance of the column and the sensitivity of the composition (or temperature) transducer.

Since there is no single tray that will be the most satisfactory for all possible disturbances, the tray selected for control, normally will only be the most suitable "optimum" tray for a certain specified disturbance. Once the "optimum" tray has been located, and the temper-

ature of the liquid on this tray is to be kept constant in spite of external disturbances, the manner of changing of the manipulative variable as a function of time to bring the column as quickly as possible back to the desired steady-state must be considered. The answer will depend on the dynamics of the column. Studies of the dynamics of distillation columns have required extensive use of large scale computing machines. The most promising methods available at present are probably:

(i) Direct solution of the mathematical equations describing the plant on an analog or digital computer.

(ii) Obtaining approximate system transfer functions from easily obtainable experimental data such as transient response, pulse response, frequency response, etc.

For a distillation column, the complexity of the differential equations is such as to require many simplifying assumptions in order to obtain solutions to the equations of the model. Because of these assumptions, the resulting mathematical model is so limiting that the second approach of using approximate, empirical transfer functions would be more attractive. The control performance of the column will be studied by simulating the column on a digital computer using the empirical models of the column and a two-mode proportional plus integral feedback controller. Combined feedback-feedforward control schemes will also be considered.

Finally, experimental tests have been carried out on the pilot-

scale distillation column located in the Department of Chemical and Petroleum Engineering at the University of Alberta to determine the applicability of such simulations in predicting the control performance of a binary distillation column.

CHAPTER II

LITERATURE SURVEY ON OPTIMUM SENSOR LOCATION

The "optimum" location of control point in a distillation column has been the subject of considerable conjecture and discussion in the technical literature. Most of the earlier work was empirical and inspired from the experience of its authors on the practical application of control (16,17,57,74). Recently, work has been done in an attempt to provide a theoretical basis for the investigation of this problem (4,60,64,79,81). The rules obtained are almost invariably based either on the sensitivity of the composition analyzer, or on the steady-state errors of the desired products, or on the control performance of the column. Needless to say, use of any design based on these approaches will require compromise before any final recommendation is made concerning the location of the control point.

Although there are different types of composition analyzers available on the market such as spectrometers, gas chromatographs, etc., the use of temperature as a means of sensing product quality is still very popular, due mainly to its very rapid response and its relatively low cost. For binary systems, temperature and pressure taken together can be used to deduce the composition, whereas, for multicomponent systems, controlling the boiling point at a given pressure does not exactly fix the composition, but it does limit changes of composition,

and it is therefore still a useful means of control.

During the late 1940's and early 1950's, as most composition analyzers or temperature indicators and recorders had poor sensitivity, measurement near or at the ends of the column was particularly discouraged by most of the authors at that time (17,57,74,75). Tivy (74) has shown by experimental results that the control of top product composition by locating the temperature sensing element in the overhead line might not be satisfactory. Indeed, unless stringent composition analyzers are available so that small variations of the sampled variable can be detected, no matter how well the overhead composition was controlled, product still varies. Williams et al (79) in 1956 investigated the effect of the sensitivity of the measuring element on the control performance of the distillation column. It was found that if the error due to the measurement of the temperature detector is greater than the expected deviation of the controlled variable, the control at this point would result in a poor control performance of the column. To overcome this problem of low sensitivity of the detector, numerous authors suggested the measurement at an intermediate tray away from the ends of the column to increase the magnitude of the signal to the controller.

Some authors emphasized the importance of the tray exhibiting a maximum in the temperature or composition gradient curve. Among them, Pyle (57) proposed that if reflux flow is used to control the temperature, the temperature sensor should be located at some tray near and above the feed tray where there is a reasonable temperature differential per tray,

on the order of 3°C to 5°C. Locating the temperature detector near the point of feed entry has the advantage that fast correction of temperature changes, as they proceed from the feed tray toward the top of the column, is possible. However, the dead time due to the liquid flow lag between the reflux valve and the detector becomes larger as the sensing location moves down the column. This time lag which causes the large phase shift in the high frequency range must be decreased in order to increase the controllability of the column. This consideration certainly led Boyd (17) and Bertrand and Jones (14) to a recommendation which suggested that a compromise should be made between the point where the temperature change per tray is maximum and the point with the least time lag. Bertrand and Jones, by performing tray-to-tray calculations on a column separating a benzene-toluene mixture, also showed that there exist two plates in the column on each side of the feed entry where the column temperature profile is steepest, and they concluded that the temperature detector should be located at one of these trays; if reflux flow is used as the manipulative variable, the sensor should be located in the rectifying section and if steam flow is used to control the temperature, the sensor should be positioned in the stripping section of the column.

On the other hand, other authors have recommended the selection of the control tray as that tray where the temperature or composition change is greatest for a given change in top product purity. The reason for this selection, as Tivy (74) explained is that at this control tray, there can be substantial changes in temperature without materially af-

fecting the product purity. Uitti (75) developed a computational approach to determine the location of these control trays and the effect of the selection of the sensing point upon the control behavior of the distillation column. The method consists of making numerous McCabe-Thiele calculations in such a way that the total number of trays and the feed tray location are held constant. The reflux flow is then varied, and for each particular reflux rate, the temperature profile (corresponding to the composition profile given by the McCabe-Thiele diagram) is drawn. Uitti showed that there exist two control trays in the column and furthermore, the trays are those located approximately in the middle of the enriching and stripping sections of the column. This conclusion applies not only for the system propane-isobutane studied, but it can also be extended to any binary system whose equilibrium x-y diagram is symmetrical. If the top product composition is to be maintained constant using reflux flow as the manipulative variable to control the temperature, the sensing point should be located at the control tray in the rectifying section. Uitti demonstrated that the overhead composition could be held within close limits while poor control of bottom product composition was observed. Uitti's method of selecting the location of the control point has found wide support from Anisimov (1), Parkins (53) and Fenske and Broughton (25). Parkins proposed a similar approach to Uitti's. Most of the calculations were done by a digital computer instead of graphically. He considered a distillation column containing 20 theoretical trays being utilized to

separate the methanol-water system. Parkins showed that the two trays which are most sensitive to reflux flow disturbances were situated two trays away from the feed tray. He concluded that in general, it is preferable to locate the sensing point at one of these trays; the sensor should be located in the enriching section in the case of reflux manipulation, and in the stripping section if steam is used as the corrective medium. Parkins also mentioned that sometimes, it might be better to accept a smaller temperature signal to the temperature controller so the sensor could be located near the ends of the column to shorten the time delay in the control system. Fenske and Broughton, who also applied Uitti's procedure, studied an industrial column separating the multicomponent mixture benzene-toluene-xylene. The temperature on an intermediate tray was maintained constant by a pressure-compensated temperature controller. It was found that the top product quality is quite acceptable even if the feed composition is allowed to vary from one half to two times the feed composition of the design case. Cardenas (21) also recommended the use of Uitti's procedure to locate the control point. Further, he pointed out that within the accuracy of experimental data, the feed composition has negligible effect upon the location of the temperature control point.

Although Uitti's method can be used to select the location of the sensing point which would give an acceptable product quality, it is not necessarily that the location of this tray would result in product with the best possible purity. In a computational study, Wood (84)

demonstrated this situation using the multicomponent system benzene-toluene-ortho, meta and para-xylene. The steady-state behavior of the column was studied for feed flow disturbances with the temperature of the liquid on an intermediate tray maintained constant by varying the reflux flow rate. Only the calculated temperatures for trays 8, 10, 14 were reported (trays are numbered from the top down). By plotting the liquid temperature on an intermediate tray versus the top product composition for different feed flow rates, it was shown that, corresponding to a decrease of 10 per cent in feed flow rate, tray 14 is the most sensitive tray. However, it was found that maintaining the liquid temperature on this tray constant would cause an offset of 80 ppm of toluene in the overhead product, whereas if the liquid temperature on tray 8, the least sensitive of all three trays considered, is held constant, a steady-state offset in the overhead composition of only 40 ppm would result. He concluded that the sensor should be located at tray 8 because use of this control tray resulted in the least offset in product purity.

An alternate approach to selecting a control point in the column is to consider the actual control performance of the column. Rose and Williams (60) studied the control behavior of a distillation column and associated feedback controller by simulation. The main objective was to determine suitable controller settings which would simultaneously keep the liquid temperature on an intermediate tray constant and result in the least offset in the overhead composition. It was demonstrated that the direct control of top product composition

is to be avoided due to a considerable delay occurring in the condenser line which would cause instability for all but very small values of the controller gain. Rose and Williams recommended that locating the sensor on the top tray, the tray nearest the reflux valve, will give the best control if the sensor is sensitive enough to detect the required range of composition variations. When the sensor is not very sensitive, locating it on a lower plate may result in more accurate control. Other authors such as Izawa and Morinaga (35) and Buckley (19) supported this criterion for selecting the control point in a distillation column. Buckley also suggested that if bottom product composition is desired, steam flow should be used as the manipulative variable and the detector should be located in the liquid line to the reboiler or in the vapor space below the bottom tray. Auns (4) investigated the control behavior of a distillation column by simulation on an analog computer. The data employed was from the column used by Gerster et al (40). This column has ten trays and feed enters at tray 5 (trays are numbered from the bottom up). Its dynamic behavior was described by a set of second order transfer functions which best fitted the experimental data given by the authors (40). Different control schemes such as feedback, combined feedforward-feedback using reflux or steam as the manipulative variable were studied. The procedure was developed with the intent of minimizing the integral of the squared error of the liquid composition on each intermediate tray by finding suitable controller settings. The recommended control tray is the tray where if the liquid composition on

this tray is kept constant in spite of disturbances in feed composition, would give the best possible product purity. It was found that best top product composition control by both feedback and instantaneous feed-forward plus feedback control schemes was achieved by manipulation of reflux flow with the sensor on tray 7. Best bottom product composition control by both feedback and instantaneous feedforward plus feedback control schemes was achieved by manipulation of steam flow with the sensor on tray 3.

One of the most interesting approaches to the problem of selecting the optimal control tray is that of Rosenbrock (64) which is based on the concept of a "disturbance function". Rosenbrock defined his disturbance as the sum of the magnitudes of the rates of change of the liquid composition on all the trays, that is:

$$D = \sum_{i=0}^{n+1} \left| \frac{d}{dt} H_i \; x_i \right|$$

where H_i and x_i are the liquid hold-up and the liquid composition on the ith tray respectively. The sum is taken over all plates, the re-boiler and the condenser. The above definition applies only to a binary distillation column, but with suitable restrictions, may be extended to include multicomponent systems. The "disturbance function", D, turns out to be very useful as a measure of the degree of departure of the system from steady-state. Rosenbrock has shown that the disturbance function constitutes a Lyapunov function for a binary system

and as such, can be used to investigate stability of the system. By an appropriate physical interpretation, a controller can be devised which tends to reduce D to zero in as short a time as possible. In some cases, the reduction in D can be accomplished by accepting deviations of the outlet compositions from their desired degrees of purity. Thus, an additional measure of the behavior is introduced and called "variation of product" and is defined as:

$$G = \sum_{i=0}^{n+1} [L_i \int_0^t \left|\frac{dx_i}{dt}\right| dt + V_i \int_0^t \left|\frac{dy_i}{dt}\right| dt]$$

where L_i is the liquid flow rate of tray i with liquid composition x_i and V_i is the vapor flow rate of tray i with vapor composition y_i. In terms of D and G, the control objective can then be stated as the reduction of D to zero in as short a time as possible with the requirement that the increase of G be kept as small as possible. This is a problem which can be approached by variational methods or by dynamic programming. Originally the problem does not appear to be tractable, however, with a few assumptions and using some geometric arguments, the requirements for the optimal control tray location may often be reduced to a relatively simple form. For example, if the number of changes of signs of $\frac{d}{dt} |H_i \, x_i|$ within the column is assumed to be known and equal at least to 2 (which is usually the case) and the values of H_i all constant, the following conclusions can be withdrawn:

(i) If the reflux flow alone is to be manipulated, in general,

the strategy is to prevent any change in composition on one of two trays where the actual liquid compositions differ by $\frac{1}{2}(x_{n+1}-x_0)$. If the major disturbance is caused by variation in feed composition, for optimal control, it is best to maintain a constant composition on the tray where the desired liquid composition is:

$$x_i = x_f \pm \frac{1}{4}(x_{n+1} - x_0)$$

where x_f, x_{n+1}, x_0 are the liquid composition at the feed tray, the condenser and the reboiler respectively.

(ii) Similar results were obtained if boil-up rate alone is used to control the distillation column, the strategy is to maintain the composition on the tray where the desired vapor composition is:

$$y_i = y_f \pm \frac{1}{4}(x_{n+1}-x_0)$$

where y_f is the vapor composition at the feed tray.
For all practical purposes, these requirements are the same as for control by means of the reflux.

In spite of all the virtues of sensing at an intermediate tray, the control of a distillation column by this method also has its disadvantages namely:

(i) The relationship between the liquid composition (or temperature) on an intermediate tray and the overhead or bottom product composition

is ambiguous.

(ii) It is well known that large variations in the composition (or temperature) in the central part of the column can occur when disturbances in product composition produced by feed composition or feed flow variations are cancelled by action of feedforward controllers. Thus, use of the liquid composition (or temperature) on an intermediate tray to generate large error signals in feedback loop can lead to serious difficulties, particularly in the presence of feedforward control.

CHAPTER III

CONTROL SCHEMES

3.1 Introduction

The best location of the sensing element for temperature control of any distillation column should be based not only on the steady-state errors in product compositions, but also on the dynamic performance of the column. Both, in turn, depend on the control scheme chosen for the control of the distillation column.

The detection of the presence of the upset can be accomplished by measuring the composition of any dependent stream in the column by means of infrared analyzers, refractometers, chromatographs, etc., or simply by means of its temperature. The correction may be carried out principally in two ways. In one scheme, the independent variable subject to upset may be measured, then when the upset occurs, action is taken to prevent its effects from reaching the process or to prepare the process ahead of time for the disturbance. Such control is known as feedforward control. Feedforward control can be quite satisfactory, but its disadvantage is that every independent variable that may affect the process must be detected and its possible effects compensated. In the second type of control, the dependent variable governing product rate or quality is measured. Then when the presence of an upset is detected by deviations of this variable from a desired value, changes

can be made in operating conditions of the process which would tend to correct the detected deviation and thus compensate for the upset. Such control is known as feedback control. Feedback control is by far the most common and must be used even in conjunction with feedforward control; theoretically, only one detecting instrument and one controller are necessary for the whole process, rather than one on each independent variable as for feedforward control. This concept of simplicity, however, suffers from two important drawbacks. First, for complex processes, one correction method can not possibly compensate for the effects of variations in several different variables, secondly, a deviation must occur in the value of the sampled dependent variable before corrective action can be taken, thus the variable can not be maintained exactly at the desired specifications. It is advantageous in some cases to couple feedforward systems to feedback loops. The resulting control system is usually known simply as a combined feedforward-feedback control system.

3.2 Literature Survey on Control Schemes

Considerable has been written on control schemes used for continuous distillation columns. Pyle (57) set down the results of experience, discussing the considerations to be made in instrumenting a column with no intermediate product stream. Boyd (16,17) presented recommendations for regulating column pressure and other variables. He also suggested a "material balance control system" to keep product compositions constant when feed flow rate changes. Control systems

for commercial distillation columns have also been reported by Lupfer and Oglesby (38) and Wherry and Berger (76). Luyben (43) has reviewed some of the many control schemes used to control complex distillation columns.

It is quite apparent that there are many types of control systems which can be utilized to operate a distillation tower. While all will work to some degree, each appears to have specific limitations, advantages and disadvantages. Any analysis of the various control system should take into account the behavior of the column itself and the effect of the control system on fractionating capacity. The present philosophy to select a control scheme for a continuous distillation column concerns itself with the following apsects:

(i) The goals of the process.

(ii) The choice of controlled and correcting variables.

(iii) Method of measurement of the quality of controlled variable.

(iv) Performance of a given control scheme.

Since the degree of separation of a distillation column bears directly on the choice of the proper control system, the goals are an integral part of the control problem. For the most part, literature dealing with the column control considers only the operational goal of the process, that is, how to design a control system which would produce a certain material within its specified purity. Recently, there has been increasing interest in the economic aspects of the control problem. Phister (54) presented a discussion that emphasized the role

of dollar return in fixing the objective of a control system. Archer (2) discussed the goal of an optimizing control scheme for maximizing the profitability of a particular distillation separation.

In choosing the controlled variables, it is necessary to be cognizant of the available degrees of freedom in the system being considered. Control is inherently more difficult as the number of degrees of freedom increases (43). Parkins (53) regarded the distillation tower as an energy system and therefore the control problem is one of regulating the energy balance of the column. He discussed basic principles and outlined some guidelines for setting up a distillation control system and presented methods of satisfying these guidelines along with illustrative control schemes. Williams (81) listed the column variables and classifed them as external independent, internal independent, semi-independent or dependent. He concluded that the problem is one of choosing which two of four internal independent variables should be controlled. The four internal independent variables for selection were shown to be the overhead product composition, the bottom product composition, the ratio of boil-up rate to feed rate and the ratio of distillate to bottom flow rate. He also noted that the most important semi-independent variable of column operation is feed plate location. The optimum location of feed plate is a function of both feed flow rate as well as feed composition. For some possible wide variations of feed rate and feed composition, reduction in column separating capacity beyond the capability of the control system to

correct may occur. Thus, some sort of automatic feed plate changes would be desirable. This idea has led Lupfer and Johnson (39) to develop an "optimum" automatic control scheme for a distillation column which does not only manipulate both reflux and steam flows but also provides for manipulation of the feed enthalpy and feed plate location. This optimizing control system has been evaluated on a large debutanizer column using the "predictive control" approach.

Another factor which should be considered in any final control scheme is the use of the analytical equipment for sensing product purity. At present, direct composition analyzers are not widely used as they are not very reliable, have a large measurement lag and operate on an intermittent cycle. It should be pointed out here that whenever composition analyzers are used, the minimum sampling rate which can be tolerated should be determined. In general, the sampling cycle permitted should be less than one half the mixing time constant for a plate in the column (81). Until the difficulties associated with sampled data control are overcome or high speed composition analyzers are developed, temperature control would be preferred. However, a pressure control system is necessary in most temperature control schemes.

A qualitative discussion and comparison of various conventional control systems which can be used to control any distillation column, binary or multicomponent with single feed stream and no sidestream draw-off follows.

(i) Control Scheme "A".

The control scheme shown in Figure 3.2-1 is the most direct scheme used to control the overhead composition by keeping the liquid temperature on an intermediate tray constant in spite of external disturbances. The signal from the temperature controller is used to adjust the distillate flow rate. The reflux flow is regulated by an averaging type controller which is used to control the liquid level in the reflux accumulator. The latter serves mainly to keep a liquid seal on the reflux and product lines and to provide disengaging space for non-condensables. A constant vapor flow is maintained by controlling the steam flow rate. The bottom flow rate is adjusted by the reboiler level controller.

Use of a large reflux drum can be a help in damping changes in flow and in providing a reservoir of high purity material for the reflux, but this causes the reflux flow to be sluggish. It has also been pointed out that the control behavior may also deteriorate because of inadequate mixing in the reflux accumulator (76). The major weakness of this control scheme is that any fluctuations in the condenser vapor rate would be propagated by the reflux accumulator level controller to the reflux stream. It has been shown that such fluctuations can be self-propagating and can lead to sustained control oscillations, especially if cold reflux is used on the column (82).

(ii) Control Scheme "B".

Figure 3.2-2 shows a control scheme commonly used on distillation

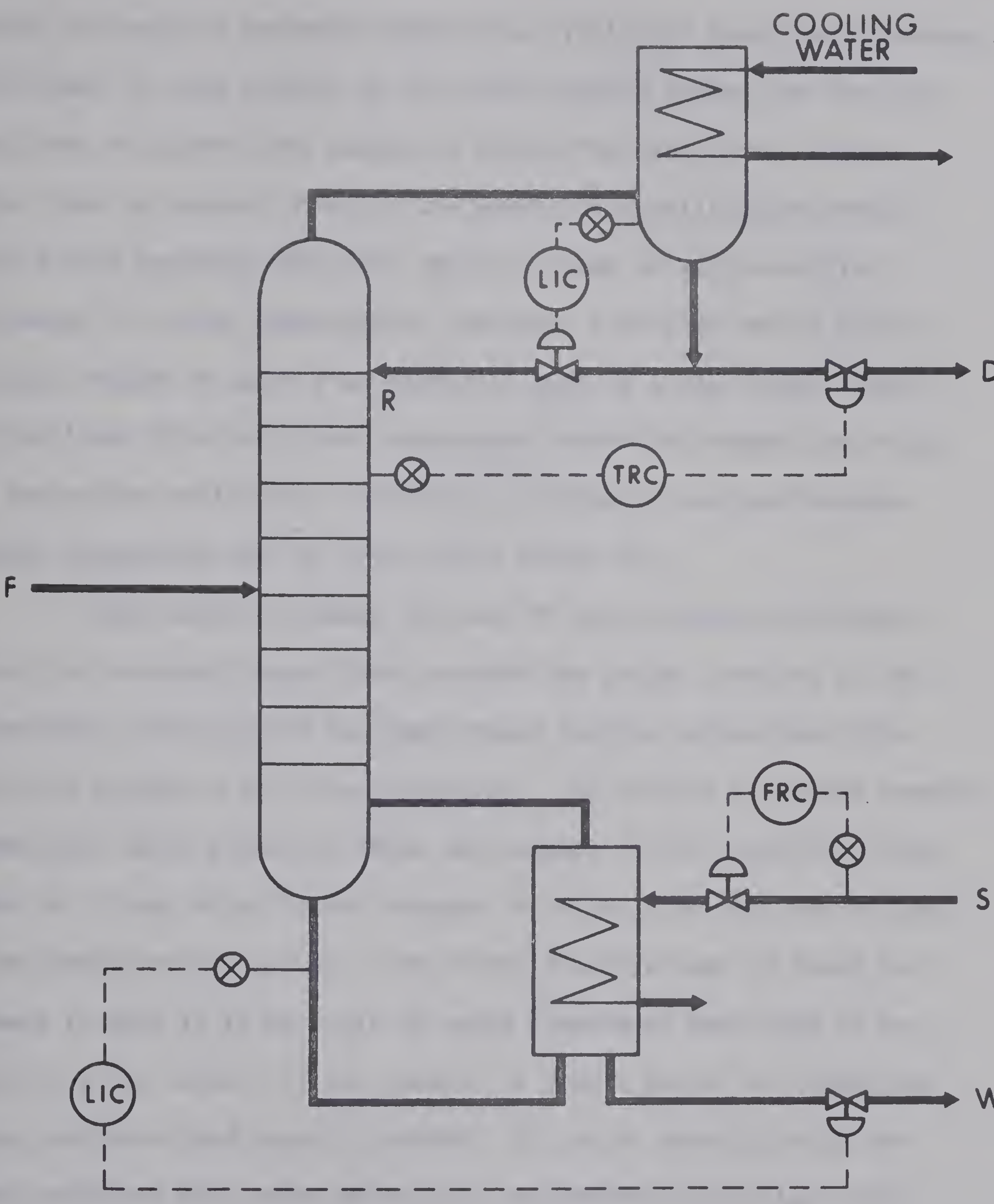


Figure 3.2-1 Temperature Control Scheme by Manipulation of Distillation Flow

columns to keep the overhead composition within its specified tolerance. This scheme is very similar to the first control scheme but care has been taken to control the amount of reflux fed back to the column rather than to control directly the amount of distillate withdrawn. Harriot (29) reported that this control scheme is very sensitive to changes in reflux temperature. Besides, with high reflux ratios, a slight change in vapor flow rate will lead to a very large change in distillate flow until the temperature controller sensed the change and varied the reflux flow. However, its steady-state performance remains unimpaired even at high reflux ratios (9).

Both control schemes "A" and "B" can provide satisfactory control of overhead composition provided the proper location of the temperature control point has been chosen and the column feed rate is not in excess of the column capacity. The control of bottom product composition using either of these two schemes is not practical since there is a large delay before changes in reflux flow rate are noticed at the bottom of the column. One of the disadvantages of these two schemes is that it is possible to waste steam when feed rate is reduced to a low value. It is, however, a simple matter to change the steam rate when feed rate is changed. It can be done by using the steam rate-feed rate ratio controller recommended by Williams (81). These control schemes also suffer from the disadvantage that they do not insure that the tower operates as a fractionating column in the event of foaming or plugging. To remedy this problem, Tivy (74) sug-

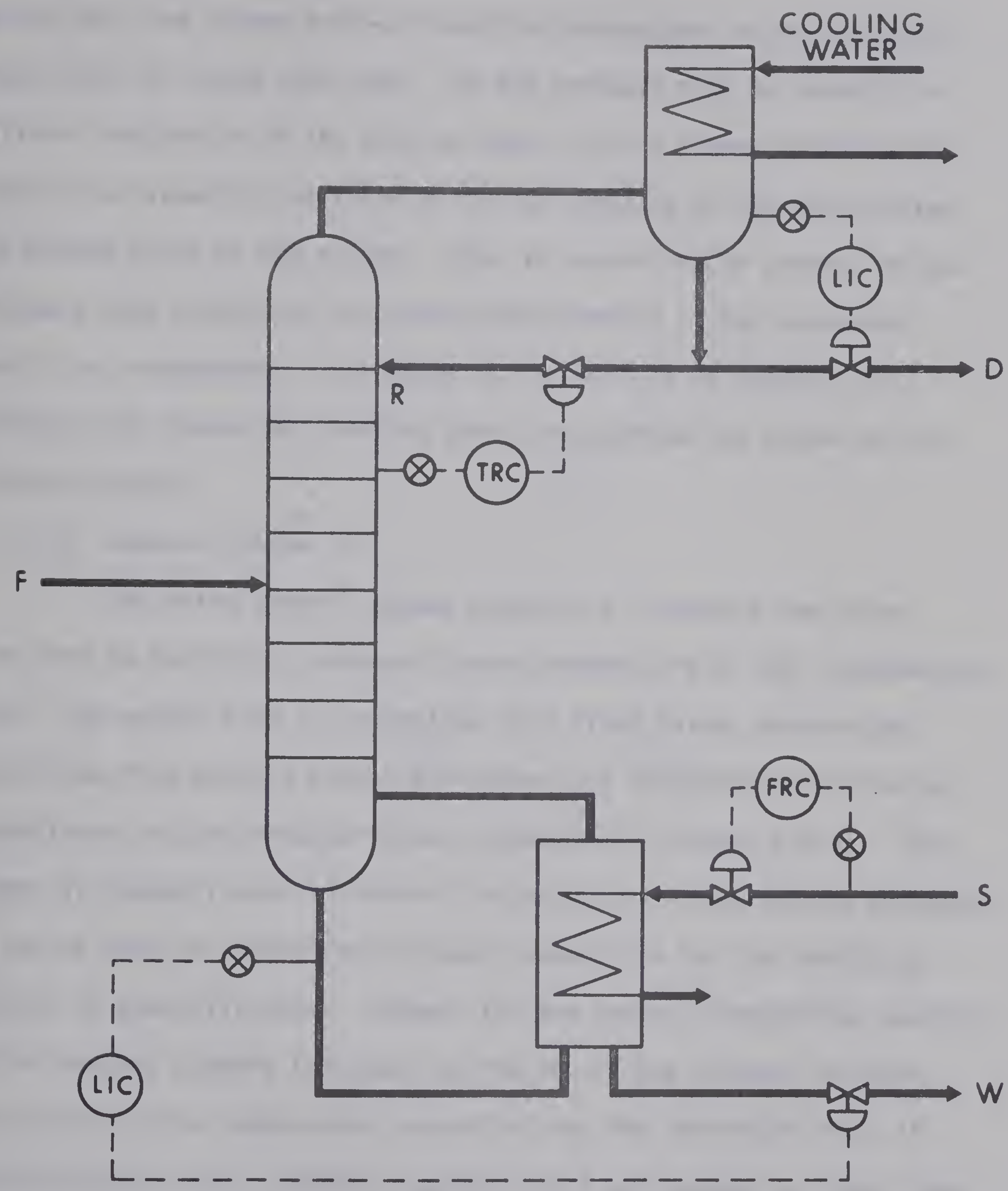


Figure 3.2-2 Temperature Control Scheme by Manipulation of Reflux Flow

gested that the proper boil-up should be maintained in the column by regulating the steam flow rate. As the pressure drop is normally a reliable indication of the boil-up rate, it is a common practice to control the steam to the reboiler by the pressure of the vapor below the bottom plate of the column. This is equivalent to control of the pressure drop across the tower when the pressure at the condenser vent is at atmospheric. Therefore it is possible to control the pressure just below the flooding point and operate the column at its maximum capacity.

(iii) Control Scheme "C"

The third control scheme consists of changing the steam flow rate to maintain a constant liquid temperature on any intermediate tray. The reflux flow is controlled at a fixed value, whereas the distillate flow and the bottom flow rates are regulated by the reflux accumulator and the reboiler level respectively (Figure 3.2-3). This scheme is normally used to control bottom product composition, although it can be used to control top product composition but the resulting control is generally poor. Indeed, for top product composition control, if the sensing element is almost at the top of the column, the wide separation of the temperature controller and the controlled flow is unsatisfactory from a dynamic standpoint and the system is slower than the first two control schemes. In such a control system, if the sensing is located close to the bottom tray, a large offset in the overhead composition would normally result.

The advantage of this arrangement is that it operates the

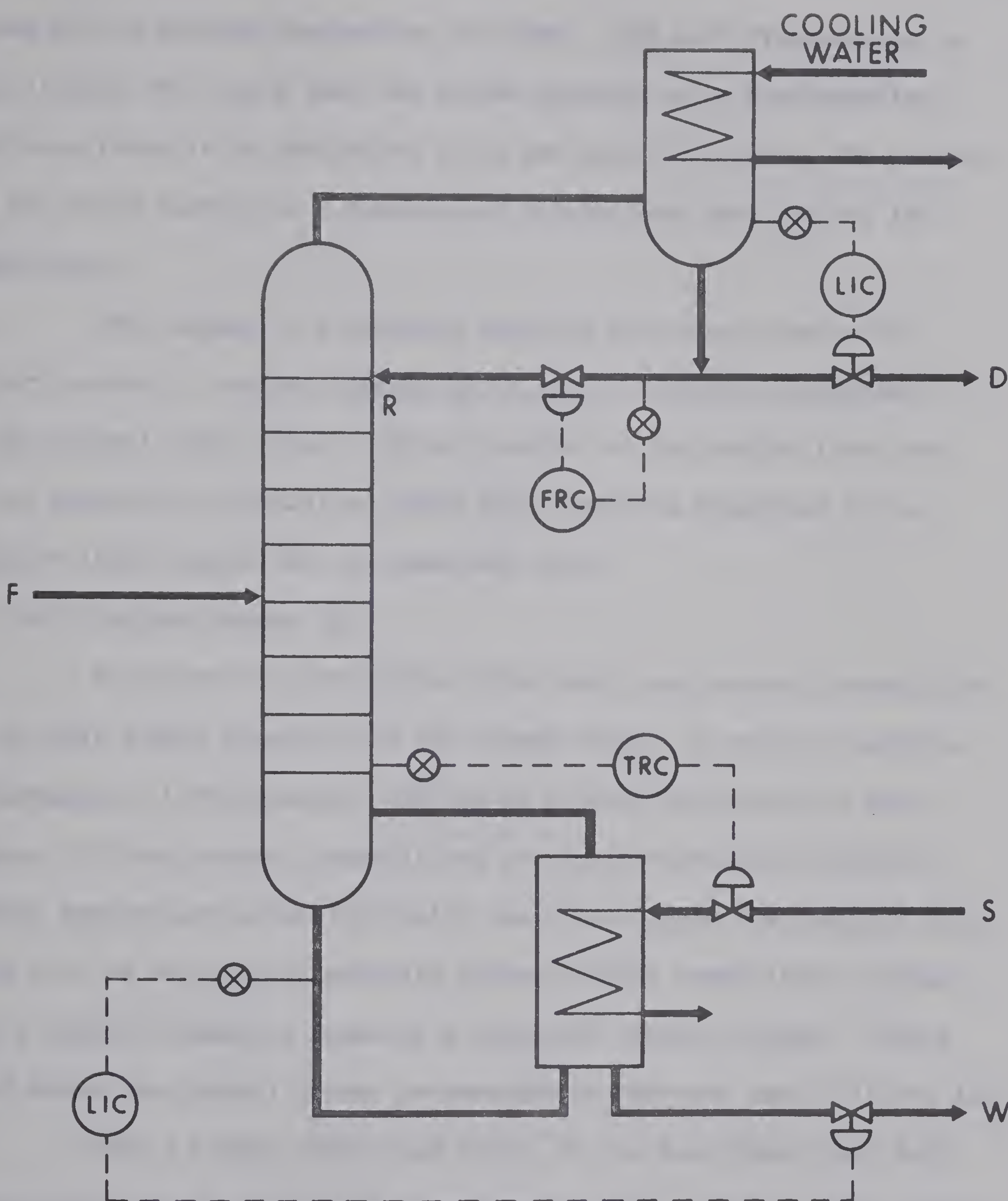


Figure 3.2-3 Temperature Control Scheme by Manipulation of Steam Flow

column with a minimum consumption of steam. The main disadvantage is that it does not insure that the column operates as a fractionating device as there is no indication as to how near to loading the column may be, since loading is a function of the boil-up rate and not the temperature.

This scheme is frequently employed and often gives satisfactory control. Another scheme, which uses a reversed arrangement of the control loops, that is direct control of the bottom flow rate by the temperature controller, with the steam flow regulated by the reboiler level controller, is sometimes used.

(iv) Control Scheme "D".

By controlling the reflux flow rate, the overhead composition can be kept almost constant (in the steady-state) in spite of external disturbances. Unfortunately, the bottom product concentration does change. If both product compositions are to be maintained constant, another temperature controller which would manipulate the reboiler heat input will be required to maintain bottom product composition constant. Such a control scheme is known as a two-point control system. Figure 3.2-4 shows the control scheme recommended by Robinson and Gilliland (59).

From a steady-state view point, it has been shown that both compositions can be controlled independently (29). Parkins (53), based on his energy or "dynamic balance" concept, saw no reason why two temperature controllers should not be used because the temperature pattern will move until the two temperature settings are satisfied. Although

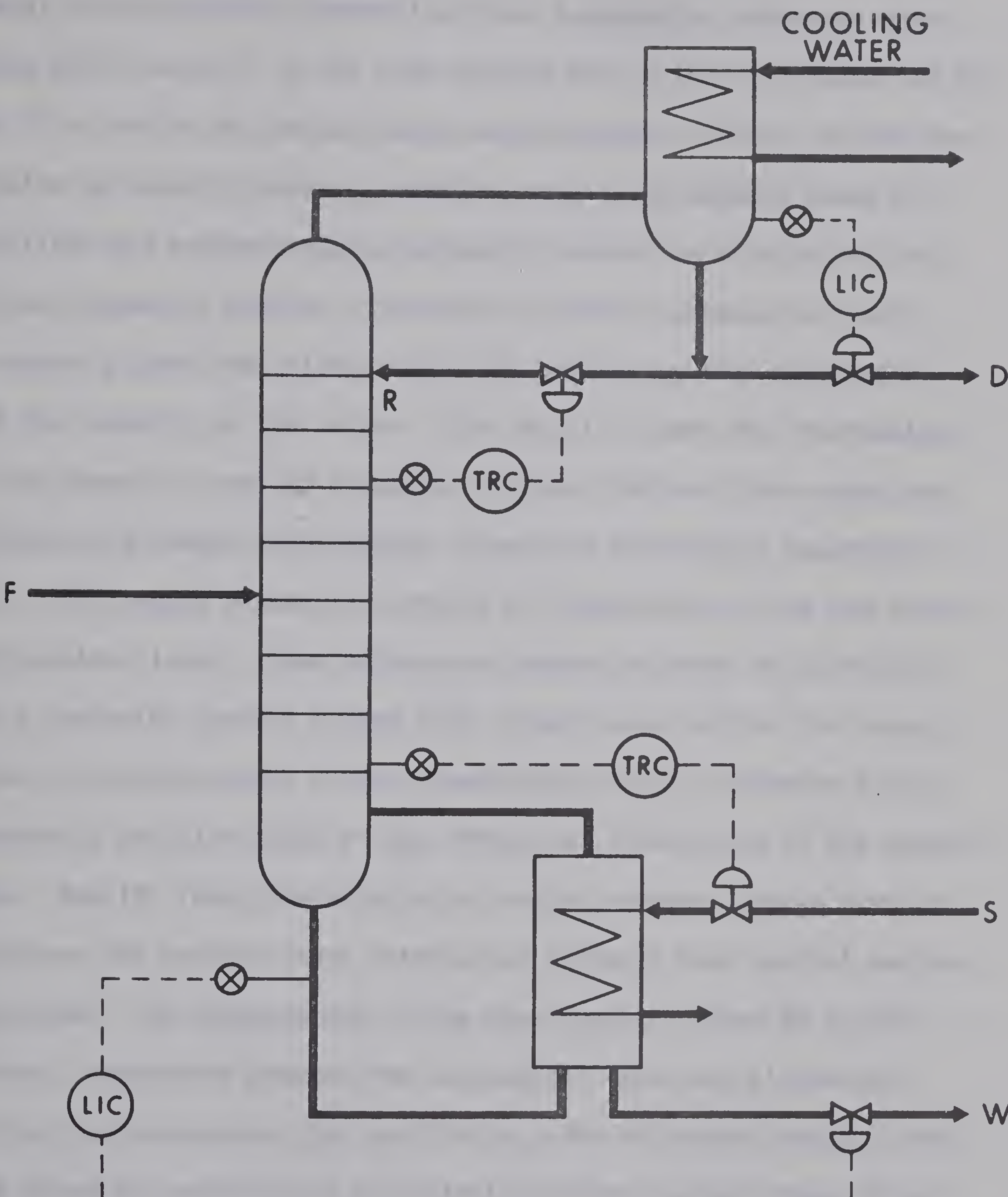


Figure 3.2-4 Two-Point Temperature Control Scheme

control of both product compositions has a potential advantage over single point control, it has been pointed out in the literature (39,64) that it is unwise to use two-point control system. First, if the feed contains an impurity having a relative volatility between those of distillate and bottom product, automatic control on both reflux and boil-up presents a problem. The reflux control operates to return the impurity down the column, while the boil-up control operates to send the impurity up the column. The result is that the intermediate boiling impurity tends to accumulate in the middle of the column and displaces the composition pattern to such an extent that separation fails. The second reason is a result of interaction of the two temperature control loops. Some columns are operating under no difficulty with a two-point control system (44), others have implied that such a scheme is unconventional or even unworkable (3,82). Rosenbrock (64) presented a detailed study of the effects of interaction of the control loops. Results from simulation on an analog computer showed that in some cases the control loops interact so strongly that control can not be achieved. By changing one of the time constants from 83 to 167 minutes, interaction between the two control loops was eliminated. This may perhaps explain the conflicting view of process control engineers about the possibility of achieving control at both ends of the column. The procedure for causing two interacting control loops to be non-interacting is known (48). Such decoupling requires a mathematical model of the process. The inability to accurately describe the dynamic

behavior of industrial columns makes this approach prohibitive at the present time.

In all the control schemes discussed so far, the split between the overhead and bottom product flows is automatically adjusted to maintain a constant temperature at some point in the column. This method of control would be effective only when the temperature fluctuations resulting from possible pressure variations are much smaller than those resulting from actual changes in composition. The sensitivity of temperature to pressure changes suggests that where temperature is to be used for distillation column control, the temperature measurement should be pressure-compensated, the only possible exception being temperature control of distillation columns at atmospheric pressure. If very close control of product purity is not necessary, the control of pressure at the top of the column would be adequate in most cases. Several control schemes have been recommended by Pyle (57), and later by Boyd (16) to control the pressure at the reflux accumulator of distillation columns operating under vacuum, atmospheric and high pressure conditions. They depend mainly on regulating the area or driving force for heat transfer in the condenser or on by-passing some gas to the reflux drum. These pressure control systems would not be very satisfactory if pressure effects can be of major importance such as distillation columns yielding high purity products, where variations in pressure due to barometric or column pressure changes may have more effect on the temperature than changes in composition. For binary sepa-

rations, column pressure dependence can be reduced by using a differential temperature control scheme or special-purpose temperature transducers. The differential temperature method to compensate for pressure variations proposed by Tivy (74) has proven to be quite satisfactory when a good reference point is available and when the differential pressure variations between the reference point and control point do not cause the control system to be unstable (45). Tivy also suggested that temperature can be used as a reliable measure of composition if a differential vapor pressure transducer is used. Buckley (19) recommended pressure compensation of temperature by measuring both temperature and pressure at the control tray and computing a "compensated temperature".

The selection of the best control scheme for a specific distillation column is governed by economic process considerations and the desired column performance. The latter generally implies feedback control of liquid temperature on an intermediate tray. Some recent articles show how steady-state calculations can be used to help select a control scheme (9,84).

Despite the numerous articles concerned with feedforward and combined feedforward-feedback binary distillation column control, the problem of feedforward plus feedback of the liquid temperature on an intermediate tray has received little attention in the literature. The only study which is pertinent to this problem is that of Luyben (45). Results from a digital simulation study of the control behavior of a 20 theoretical tray distillation column showed that feedforward plus feed-

back control provided effective control using an intermediate control tray. Indeed, with the proper feedforward controller transfer functions, steady-state errors in product compositions were eliminated, while addition of feedforward control reduced the interaction between the two feedback loops in the case of the two-point control system.

3.3 Control Schemes Evaluated

In this investigation, control schemes "B" and "C" have been evaluated for disturbances in feed conditions by digital simulation and experimental tests. In the experimental tests, care was taken to ensure that the only disturbance to the column was feed flow rate. As a cold feed condenses some vapor at the feed plate which leads to different fractionating capacity, feed temperature control was employed to keep any feed temperature disturbances from entering the system. Steam flow as regulated by a feedback temperature controller was used to maintain feed temperature constant at slightly below its boiling point in spite of variations in feed flow rate. A similar control loop was employed to maintain constant reflux temperature. Effects of barometric pressure on the controlled temperature can be reduced by using a simple pressure control scheme. The pressure in the condenser was kept at nearly atmospheric conditions by varying the flow rate of cooling water. A large vent was also located at the condenser to keep the condenser at substantially the same pressure regardless of the load on the column.

A schematic representation of the column and the principal control loops investigated is shown in Figures 3.3-1 and 3.3-2.

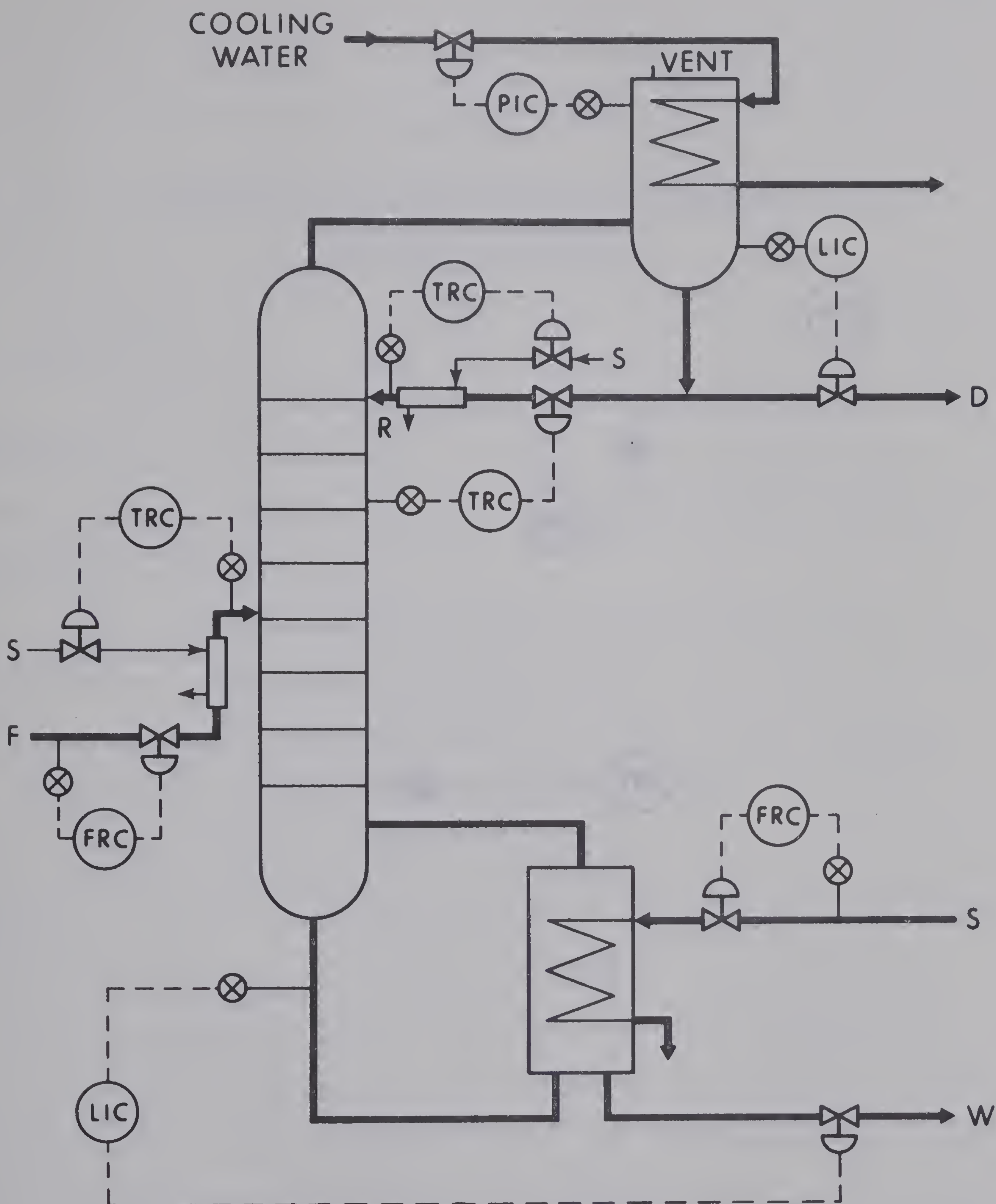


Figure 3.3-1 Evaluated Control Scheme by Manipulation of Reflux Flow

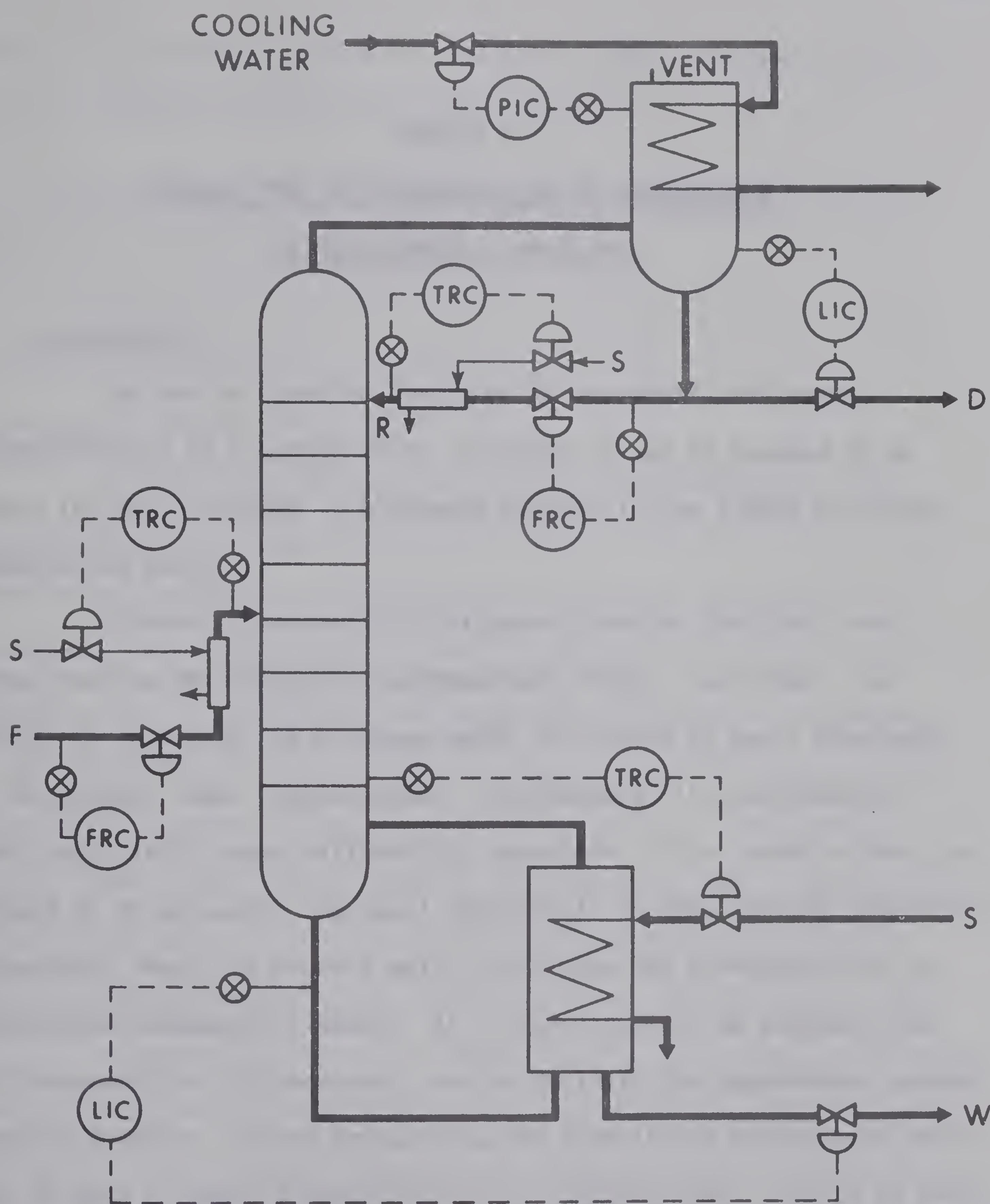


Figure 3.3-2 Evaluated Control Scheme by Manipulation of Steam Flow

CHAPTER IV

METHODS FOR THE DETERMINATION OF APPROXIMATE SYSTEM TRANSFER FUNCTIONS

4.1 Introduction

The use of transfer functions to represent the dynamic characteristics of a system which is linear or can be assumed to be linear for small changes is extremely popular in the fields of process dynamics and control.

In order to arrive at a rigorous transfer function, the system must be described with mathematical rigour, but often, the ability to formulate the rigorous model is limited by basic knowledge of the process under consideration. Furthermore, this mathematical model must yield linear differential equations if the transfer function concept is to be used. The usual approach is to make certain simplifying assumptions about the process which facilitate the formulation of an approximate mathematical model. It is then possible to proceed with the linearization, if necessary, and to evaluate the approximate system transfer function. Quite frequently, the simplifying assumptions which must be made in model formulation are so limiting that it would be just as appropriate to start with an empirical transfer function determined from transient or frequency response data.

Methods of obtaining an approximate empirical transfer function

from easily obtainable data are to be considered. Transient response, pulse and frequency response data are utilized.

4.2 Literature Survey on Different Methods for the Determination of Approximate System Transfer Functions

The construction of an empirical transfer function includes methods of determining the parameters of the model from both the time-domain and frequency-domain data.

To determine the transfer function from time-domain data, it is necessary to derive an analytical function in terms of the parameters of the transfer function in such a way that the response curve generated by the model comes as close as possible to the true transient response. Here the method of least squares fitting may be regarded as the best approach available. Numerous least squares fitting procedures have appeared in the literature, but two of the more useful methods are the ones developed by Powell (55,56) and Rosenbrock (63). Rosenbrock's method can be used for both constrained and unconstrained searches, whereas Powell's method is only applicable for unconstrained searches.

Determination of the transfer function from frequency response data has received wide attention in the literature (5,8,22,24,28,36,37, 66,67,70,71). One of the most complete accounts to date is contained in the book by Chen and Haas (23). Some of the methods developed used a graphical procedure (5,28,66) to determine the transfer function coefficients. Graphical methods have a distinct advantage in that the calculations can be carried out by hand with a reasonable time require-

ment, though they have certain deficiencies regarding accuracy and general applicability. For complicated cases or whenever a large amount of data is involved, analytical methods must be used. Most of these methods used least squares fitting techniques to approximate the frequency curves (8,24,36,37,67,72). Use of a digital computer is foreseen for most cases.

4.3 Theory

The transfer function G(s) for a time invariant, linear system incorporating no pure time delay is usually expressed by a ratio of two polynomials in s, that is:

$$G(s) = \frac{b_m s^m + b_{m-1} s^{m-1} + \ldots + b_1 s + b_0}{a_n s^n + a_{n-1} s^{n-1} + \ldots + a_1 s + a_0} \qquad (4.3\text{-}1a)$$

where m and n are the degree of the numerator and denominator respectively and $b_k (k=0,1,2,\ldots,m)$ and a_j $(j=0,1,2,\ldots,n)$ are real constant coefficients.

In the frequency domain, the transfer function G(s) can be expressed as:

$$G(j\omega) = \frac{(b_0 - b_2\omega^2 + \ldots) + j\omega(b_1 - b_3\omega^2 + \ldots)}{(a_0 - a_2\omega^2 + \ldots) + j\omega(a_1 - a_3\omega^2 + \ldots)} \qquad (4.3\text{-}1b)$$

In practice, for most cases, it is possible to represent any system by simple, low order transfer functions with or without time delays such as first, second or third order transfer functions.

For a first order system, the representation is:

$$G(s) = \frac{K}{\tau_1 s+1} \; e^{-\tau_D s} \tag{4.3-2}$$

For a second order system, the representation is:

$$G(s) = \frac{K}{(\tau_1 s+1)(\tau_2 s+1)} \; e^{-\tau_D s} \tag{4.3-3}$$

Similarly, for a third order system,

$$G(s) = \frac{K}{(\tau_1 s+1)(\tau_2 s+1)(\tau_3 s+1)} \; e^{-\tau_D s} \tag{4.3-4}$$

where K = the system gain

τ_D = the time delay in the system

τ_1, τ_2, τ_3 = the system time constant (s)

The general strategy to be used in arriving at an approximate transfer function from experimental data is as follows:

(i) Assume that the system can be adequately represented by a simple model with a transfer function given by equation (4.3-2), (4.3-3) or (4.3-4). In the general case where equation (4.3-1a) is used to represent the dynamics of the system, the degree of the numerator and denominator must be assumed.

(ii) Determine the time delay in the system, if there is any.

(iii) Curve fit the time-domain data or the frequency-domain

data using appropriate search technique. Frequency response data can be obtained either by pulse testing or direct frequency response experimentation.

(iv) Perform a statistical test to obtain the simplest transfer function which adequately represents the system.

4.3.1 Determination of the System Time Delay

Theoretically, the time delay in any system can be determined simply by shifting the zero-time to the point of the first observable deviation in the output signal. The magnitude of this shifting determines τ_D as defined in equations (4.3-2), (4.3-3) and (4.3-4). In practice, due the noise present in actual processes, it is not always possible to determine with reasonable accuracy the time of the first observable deviation in the output signal. To overcome this problem, Oldenbourg and Sartorius (50) developed a simple method which can be used to determine the time delay in any actual process from its transient response. The method is illustrated by Figure 4.3-1. The procedure is outlined as follows:

(i) Draw a tangent to the transient response at the inflection point I. The intersection of this tangent and the horizontal axis of the curve occurs at the point R. At this point, the value of the actual transient response is PR.

(ii) Point Q which has the value QR = 2.718 x PR is located on the graph.

(iii) A line parallel to the tangent through the point Q locates the equivalent dead time of the process.

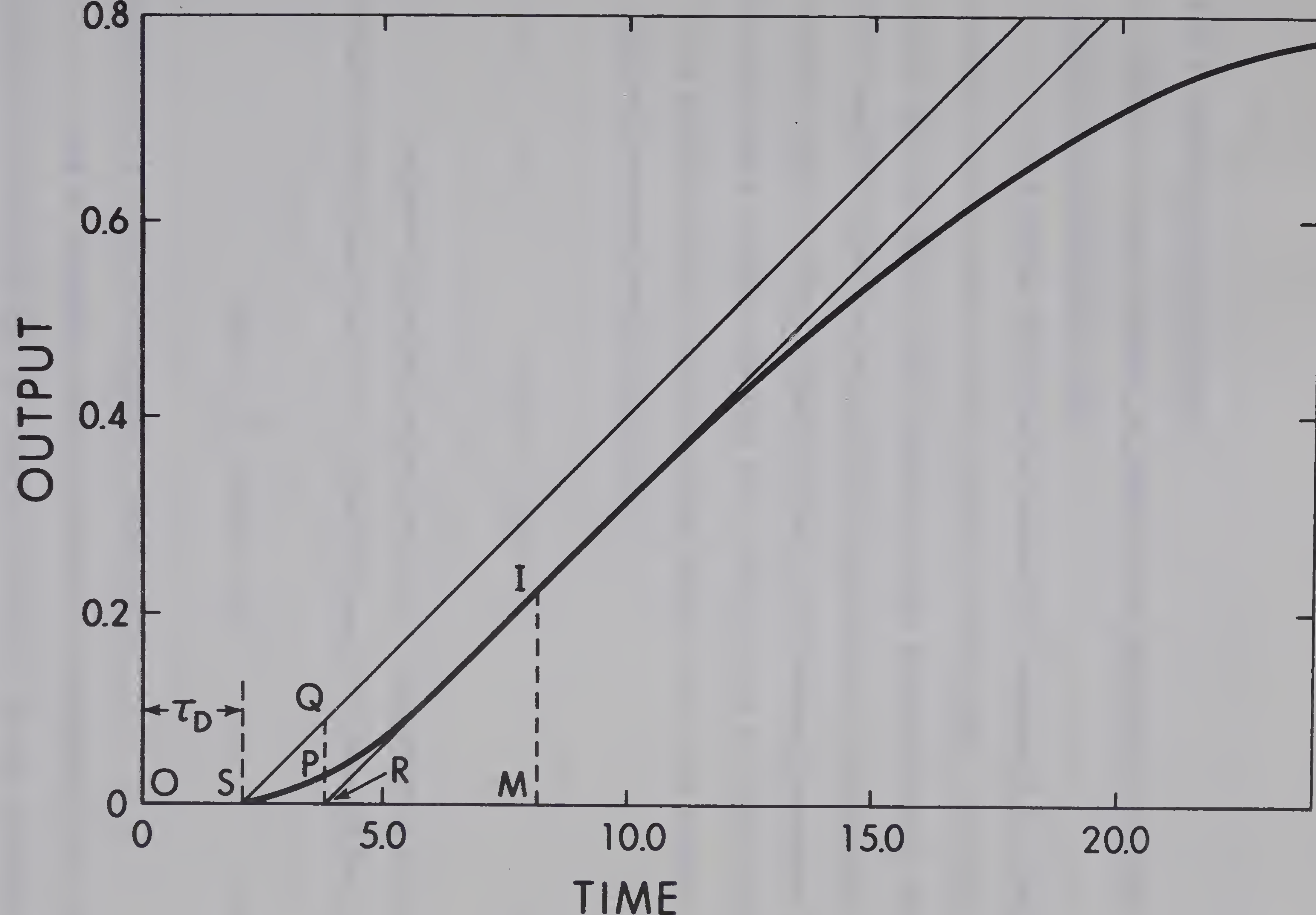


Figure 4.3-1 Determination of the Time Delay from the Transient Response

4.3.2 Curve Fitting Techniques

A. Outline of the procedure to determine an approximate transfer function from time-domain data.

If a system which can be adequately represented by simple transfer function such as first, second or third order, is excited with a step function or with a pulse of known functional form, then it is possible to derive an analytical expression of the transient response $y(\underline{p},t)$ for the system in terms of the unknown parameters $\underline{p}$ of the assumed transfer function (i.e. the gain and the time constant(s)). At any specific time t, the error $e_i(\underline{p})$ between the ideal response $y_i(\underline{p})$ and the experimental data u_i is:

$$e_i(\underline{p}) = y_i(\underline{p}) - u_i \tag{4.3-5}$$

In order to establish the best set of parameters $\underline{p}$ of the system transfer function, it is logical to seek a minimum of the function:

$$F(\underline{p}) = \sum_{i=1}^{n} (y_i(\underline{p}) - u_i)^2 \tag{4.3-6}$$

where $i = 1,2,\ldots,n$; n = number of data points.

One of the most convenient methods of determining the least value of the function $F(\underline{p})$ in equation (4.3-6) is the one developed by Rosenbrock. It has the advantages that the knowledge of the partial derivatives of the function $F(\underline{p})$ are not needed and a set of constraints

of the parameters to be optimized can be inserted in the calculations without any difficulty. Constraints are necessary to ensure that all physically unrealizable solutions are eliminated.

The Rosenbrock method is essentially an extension of the hill-climbing method. To determine the least value of equation (4.3-6), successive evaluations of the values of $F(\underline{p})$ are compared and a set of rules defines the action to be taken according to the outcome of the comparison. The two difficulties which have to be met in evaluating successive values of $F(\underline{p})$, i.e. $F(p^{(1)})$ and $F(\underline{p}^{(2)}) = F(\underline{p}^{(1)} + \underline{\xi}^{(1)})$ are:

(i) Determination of the directionsof $\underline{\xi}^{(1)}$

(ii) Determination of the lengths of $\underline{\xi}^{(1)}$

To overcome these difficulties, Rosenbrock suggested the following procedure.

A set of ℓ orthogonal unit vectors $\underline{v}_1$, $\underline{v}_2$, ..., $\underline{v}_\ell$ and a set of step lengths d_1, d_2, ..., d_ℓ are stored in the computer (ℓ is the number of unknown parameters to be optimized). The successive changes in parameters $\underline{p}$ are $d_1\underline{v}_1$, $d_2\underline{v}_2$, ..., $d_\ell\underline{v}_\ell$. After each evaluation of the function $F(\underline{p})$, the new value $F(\underline{p}+\underline{\xi})$ is compared with the best value F_0 so far obtained. If $F(\underline{p}+\underline{\xi}) \leq F_0$, then the solution is moved forward to $\underline{p} + \underline{\xi}$ and the value of F_0 is replaced by $F(\underline{p}+\underline{\xi})$. On the other hand, if $F(\underline{p}+\underline{\xi}) > F_0$, the current set of parameters $\underline{p}$ and the value of F_0 are maintained at their original values. After each evaluation of $F(\underline{p})$, the corresponding step lengths $\underline{d}$ (so that $\underline{d} = (d_1, d_2, ..., d_\ell)$)

are modified. If the evaluation is successful, the values of $\underline{d}$ are trebled. If it was unsuccessful, $\underline{d}$ is multiplied by -1/2. These values, 3 and - 1/2, were selected by Rosenbrock, on the basis of computational work, as those that give good efficiency in a moderately difficult problem (63). The search is made along one direction at a time and the procedure is continued until a successful step has been made in the direction of $\underline{v}_k$, followed by a failure for every direction k. Thus, the procedure is not interrupted until each step length d_k has first adjusted itself to the correct magnitude. When this happens, the procedure is interrupted and the axes $\underline{v}_k$ are replaced by a new set of orthogonal unit vectors obtained by using the Gram-Schmidt orthogonalization procedure (77).

For further details of this method, the book by Rosenbrock and Storey (65) should be consulted.

To insert the limits on the parameters to be optimized, it is sufficient to ensure that the constraints are not transgressed. Indeed, if a parameter $\underline{p}_k$ is restricted to lie between a lower limit a and an upper limit b, and at any stage of the iteration procedure, the Rosenbrock method calls for $p_k < a$ or $p_k > b$, then p_k will be temporarily fixed at either a or b and only the remaining parameters are varied.

A computer program was written to determine approximate transfer functions from time-domain data by the Rosenbrock search technique. Program listings appear in Appendix B.

B. Outline of the methods used to determine an approximate transfer function from frequency-domain data.

Fitting a transfer function to time-domain data suffers from the disadvantage that the procedure is only applicable when the transient response of the system can be described adequately by an analytical expression. This condition is satisfied only when the transfer function is simple and the excitation applied to the system has a known functional form. The latter condition can not generally be satisfied in practice because of the difficulties in producing exact forcing functions. Therefore, sometimes, it is necessary to be able to determine the transfer function from frequency response data. The present investigation is restricted only to the methods which can be easily programmed on a digital computer. They are the methods of Bailey and Law (8), of Chen and Philip (22), of Levy (37) and of Staffin and Staffin (70). Also investigated here is the determination of transfer function coefficients using Rosenbrock's search technique in the frequency domain. Computer programs were written for each of these methods. Program listings appear in Appendix B.

a. Bailey and Law Technique

The Bailey and Law method is a regression technique for fitting the data by an equation of the form:

$$y_i = f(u_{1i}, u_{2i}, \ldots, u_{ri}, p_1, p_2, \ldots, p_\ell) \tag{4.3-7}$$

where y_i = the dependent variable

u_{ji} = the independent variable

p_k = the unknown parameters to be optimized

$j = 1,2,\ldots,r$ r = number of independent variables

$k = 1,2,\ldots,\ell$ ℓ = number of unknown parameters

$i = 1,2,\ldots,n$ n = number of data points

The method of least squares fitting requires that in order to obtain a set of parameters p_k in equation (4.3-7) which best fits the experimental data, it is proper to seek an unrestricted minimum of the following expression:

$$S_T = \sum_{i=1}^{n} S_i^{\,2} = \sum_{i=1}^{n} (y_i - \phi_i)^2 \tag{4.3-8}$$

where $i = 1,2,\ldots,n$ n = number of data points

y_i = value of the model determined by equation (4.3-7)

ϕ_i = experimental data

If the function, f, in equation (4.3-7) is non-linear in the parameters p_k, minimization of equation (4.3-8) is a non-linear problem. Therefore, one of the possible means for its solution is linearization by means of a Taylor series expansion. For the (j+1)th iteration, the following expression is obtained by truncating all but the linear terms:

$$f^{(j+1)} = f^{(j)} + \left[\frac{\partial f}{\partial p_1}\right]^{(j)} \Delta p_1 + \left[\frac{\partial f}{\partial p_2}\right]^{(j)} \Delta p_2 + \ldots + \left[\frac{\partial f}{\partial p_\ell}\right]^{(j)} \Delta p_\ell \tag{4.3-9}$$

where superscript (j) refers to the iteration j and

$$\Delta p_k = p_k^{(j+1)} - p_k^{(j)} \tag{4.3-10}$$

To seek an unrestricted minimum of equation (4.3-8), the following equation must be satisfied:

$$\frac{\partial \sum_{i=1}^{n} S_i^2}{\partial p_k} = 0 \tag{4.3-11}$$

The fitting procedure, then, involves solving ℓ simultaneous linear equations which can be written in abbreviated matrix form as:

$$\underline{\underline{Z}} \times \underline{B} = \underline{C} \tag{4.3-12}$$

or more explicitly,

$$\begin{vmatrix} \Sigma Z_1^{(j)} Z_1^{(j)} & \Sigma Z_1^{(j)} Z_2^{(j)} & \cdots & \Sigma Z_1^{(j)} Z_\ell^{(j)} \\ \Sigma Z_2^{(j)} Z_1^{(j)} & \Sigma Z_2^{(j)} Z_2^{(j)} & \cdots & \Sigma Z_2^{(j)} Z_\ell^{(j)} \\ \vdots & \vdots & & \vdots \\ \Sigma Z_\ell^{(j)} Z_1^{(j)} & \Sigma Z_\ell^{(j)} Z_2^{(j)} & \cdots & \Sigma Z_\ell^{(j)} Z_\ell^{(j)} \end{vmatrix} \times \begin{vmatrix} \Delta p_1^{(j)} \\ \Delta p_2^{(j)} \\ \vdots \\ \Delta p_\ell^{(j)} \end{vmatrix} = \begin{vmatrix} C_1^{(j)} \\ C_2^{(j)} \\ \vdots \\ C_\ell^{(j)} \end{vmatrix} \tag{4.3-13}$$

where $\Sigma = \sum_{i=1}^{n}$ (summation over all data points)

$$Z_k^{(j)} = \left[\frac{\partial f}{\partial p_k}\right]^{(j)}$$

$$C_k^{(j)} = \sum_{i=1}^{n} [S_i (Z_k)_i]^{(j)}$$

$\Delta p_k^{(j)}$ is given by equation (4.3-10)

$\underline{\underline{Z}}$ = the matrix of Z_{jk}'s in equation (4.3-12)

$\underline{B}$ = the vector of Δp_k's in equation (4.3-12)

$\underline{C}$ = the vector of C_k's in equation (4.3-12)

From equation (4.3-12), $\underline{B}$ can be calculated by:

$$\underline{B} = \underline{\underline{Z}}^{-1} \times \underline{C} \tag{4.3-14}$$

The values of Δp_k in the vector $\underline{B}$ will be found by solving equation (4.3-14) and new values of $p_k^{(j+1)}$ for the next iteration (j+1) will be computed from equation (4.3-10). The procedure is repeated until the corrections Δp_k become negligibly small.

However the above procedure will normally lead to a divergence unless the original starting values of p_k are very nearly equal to the correct values. To overcome this problem, Bailey and Law suggested the following modifications of the above technique which would ensure convergence if there is a unique solution:

(i) Introduce a new variable D_T which is defined by the following equation:

$$D_T = \sum_{k=1}^{n} (\Delta p_k)^{(j)} C_k^{(j)} \tag{4.3-15}$$

D_T must be positive if the direction is toward a minimum. If D_T is negative, the signs of all Δp_k must be changed.

(ii) Define

$$\Delta S_a^{\,2} = [S_a^{\,2}]^{(j)} - [S_a^{\,2}]^{(j+1)} \tag{4.3-16}$$

$\Delta S_a^{\,2}$ must be positive if the iteration procedure is converging. If $\Delta S_a^{\,2}$ is negative, then the present values of the corrections Δp_k must be restricted according to the relation:

$$\Delta p_k^{(j+1)} = \alpha \cdot \Delta p_k^{(j)} \tag{4.3-17}$$

where α is the fraction that the changes are restricted.

(iii) Even if $\Delta S_a^{\,2}$ is positive, the convergence might be relatively slow. The speed of convergence can be improved by using the following criterion:

$$\Delta S_a^{\,2} - \beta D_T(2\alpha - \alpha^2) \geq 0 \tag{4.3-18}$$

Bailey and Law suggested that values of $\alpha = 0.5$ and $\beta = 0.25$ are generally suitable for maximum progress toward the minimum.

An examination of the above procedure suggests that the Bailey and Law technique can be applied to fitting the transfer function forms of equations (4.3-2), (4.3-3) and (4.3-4) since the magnitude

ratios and the phase angles corresponding to these transfer functions can be described by analytical expressions of the form of equation (4.3-7).

As an illustration, for a second order transfer function with unit gain and no time delay; the magnitude ratio can be expressed as:

$$|G| = [(\tau_1^2\omega^2+1)(\tau_2^2\omega^2+1)]^{-1/2} \tag{4.3-19}$$

Then be letting

$$y_i = |G|_i$$
$$u_{1i} = \omega_i = u_i$$
$$p_1 = \tau_1^2$$
$$p_2 = \tau_2^2$$

The following expressions are obtained:

$$y_i = [(p_1u_i{}^2+1)(p_2u_i{}^2+1)]^{-1/2} \tag{4.3-20}$$

$$Z_1 = -\frac{1}{2}(u_i{}^2+p_2u_i{}^4)\ y_i{}^3 \tag{4.3-21}$$

$$Z_2 = -\frac{1}{2}(u_i{}^2+p_1u_i{}^4)\ y_i{}^3 \tag{4.3-22}$$

With these equations, it is then possible to determine for the values of p_1, p_2 by the Bailey and Law technique.

The corresponding equations for other representations may be obtained in a similar manner.

b. Chen and Philip Technique

To determine the transfer function using the Chen and Philip method, it is necessary to express the assumed transfer function in the form:

$$G(s) = A_0 + A_1\left(\frac{1-s}{1+s}\right) + A_2\left(\frac{1-s}{1+s}\right)^2 + \ldots + A_n\left(\frac{1-s}{1+s}\right)^n \qquad (4.3\text{-}23)$$

The basis of this method is the determination of the coefficients A_0, A_1, A_2, ..., A_n. To determine the values of A_k, the following technique was developed by Chen and Philip.

With the use of a bilinear transformation:

$$e^{-j\theta} = \left.\frac{1-s}{1+s}\right|_{s\to j\omega} \qquad (4.3\text{-}24)$$

G(s) can be transformed from the s domain to the θ domain. Indeed,

$$G(\theta) = A_0 + A_1 e^{-j\theta} + A_2 e^{-j2\theta} + \ldots + A_n e^{-jn\theta} \qquad (4.3\text{-}25)$$

Since $G(\theta)$ is a complex function, it can be separated into

its real and imaginary parts:

$$G(\theta) = R(\theta) + j\, I(\theta) \tag{4.3-26}$$

Equating the $R(\theta)$ with the real part of the right-hand side of equation (4.3-25) yields:

$$R(\theta) = A_0 + A_1\cos\theta + A_2\cos 2\theta + \ldots + A_n\cos n\theta \tag{4.3-27}$$

If the values of $R(\theta)$ are available, the values of A_k can be determined by a Fourier series expansion.

$$A_k = \frac{1}{\pi}\int_0^{2\pi} R(\theta)\cos k\theta\, d\theta \tag{4.3-28}$$

Since an analytical expression of $R(\theta)$ is not normally available, the integral in equation (4.3-28) must be computed numerically. The values of $R(\theta)$ can be determined from the real part function $R(\omega)$ of the transfer function $G(j\omega)$ from the frequency response data by using the following transformation.

$$\theta = 2\tan^{-1}\omega \tag{4.3-29}$$

Once the values of A_k are determined from equation (4.3-28) they are substituted back into the original transfer function (4.3-23).

C. Levy Technique

Levy's method of fitting transfer function to frequency response data is an extension of the least squares fitting process. Assuming that the frequency response data for any system can be represented by equation (4.3-1b), Levy first separated the numerator and denominator into real and imaginary parts:

$$G(j\omega) = \frac{[b_0-b_2\omega^2+b_4\omega^4-\ldots] + j\omega[b_1-b_3\omega^2+b_5\omega^4-\ldots]}{[a_0-a_2\omega^2+a_4\omega^4-\ldots] + j\omega[a_1-a_3\omega^2+a_5\omega^4-\ldots]} \qquad (4.3\text{-}30)$$

$$= \frac{N(\omega)}{D(\omega)}$$

Suppose further the existence of a function $F(j\omega)$ that represents exactly the data points of the experimental frequency curve, $F(j\omega)$ will also have real and imaginary parts as given by:

$$F(j\omega) = R(\omega) + j\,I(\omega) \qquad (4.3\text{-}31)$$

At any specific value of frequency ω_i, the error in fitting is then,

$$e(\omega_i) = F(j\omega_i) - G(j\omega_i) \qquad (4.3\text{-}32a)$$

$$= F(j\omega_i) - \frac{N(\omega_i)}{D(\omega_i)} \qquad (4.3\text{-}32b)$$

Multiplication of both sides of equation (4.3-32b) by $D(\omega_i)$ gives:

$$e(\omega_i)\ D(\omega_i) = F(j\omega_i)\ D(\omega_i) - N(\omega_i) \tag{4.3-33}$$

Equation (4.3-33) may then be separated into real and imaginary parts as

$$e(\omega_i)\ D(\omega_i) = A(\omega_i) + jB(\omega_i) \tag{4.3-34}$$

and it follows that the magnitude of this expression is

$$|D(\omega_i)\ e(\omega_i)| = \sqrt{[A(\omega_i)]^2 + [B(\omega_i)]^2} \tag{4.3-35}$$

Levy's method consists of defining a function E as defined by:

$$E = \sum_{i=1}^{n} [A(\omega_i)]^2 + [B(\omega_i)]^2 \tag{4.3-36}$$

where n is the number of data points.

The unknown coefficients a_j and b_k in equation (4.3-1b) are now evaluated by minimizing E. For least squares fitting, it is necessary to minimize E by setting the partial derivatives of E with respect to each of the coefficients a_j and b_k equal to zero. This results in a

set of linear simultaneous equations which may be solved for the desired coefficients. By some mathematical transformations, Levy arrived at the following set of linear equations, by assuming that $a_0 = 1$.

$$\lambda_0 b_0 - \lambda_2 b_2 + \lambda_4 b_4 - \lambda_6 b_6 + \cdots$$
$$+ T_1 a_1 + S_2 a_2 - T_3 a_3 - S_4 a_4 + T_5 a_5 + \cdots = S_0$$

$$\lambda_2 b_1 - \lambda_4 b_3 + \lambda_6 b_5 - \lambda_8 b_7 + \cdots$$
$$- S_2 a_1 + T_3 a_2 + S_4 a_3 - T_5 a_4 - S_6 a_5 + \cdots = T_1$$

$$\lambda_2 b_0 - \lambda_4 b_2 + \lambda_6 b_4 - \lambda_8 b_6 + \cdots$$
$$+ T_3 a_1 + S_4 a_2 - T_5 a_3 - S_6 a_4 + T_7 a_5 + \cdots = S_2$$

$$\lambda_4 b_1 - \lambda_6 b_3 + \lambda_8 b_5 - \lambda_{10} b_7 + \cdots$$
$$- S_4 a_1 + T_5 a_2 + S_6 a_3 - T_7 a_4 - S_6 a_5 + \cdots = T_3 \qquad (4.3\text{-}37)$$

$$\vdots$$

$$T_1 b_0 - S_2 b_1 - T_3 b_2 + S_4 b_4 - \cdots$$
$$+ U_2 a_1 - U_4 a_3 + U_6 a_5 - U_8 a_7 + \cdots = 0$$

$$S_2 b_0 + T_3 b_1 - S_4 b_2 - T_5 b_3 + \cdots$$
$$+ U_4 a_2 - U_6 a_4 + U_8 a_6 - U_{10} a_8 + \cdots = U_2$$

$$T_3b_0 - S_4b_1 - T_5b_2 + S_6b_3 + \cdots$$

$$+ U_4a_1 - U_6a_3 + U_8a_5 - U_{10}a_7 + \cdots = 0$$

$$\vdots$$

where

$$\lambda_j = \sum_{i=1}^{n} \omega_i^{\,j}$$

$$S_j = \sum_{i=1}^{n} \omega_i^{\,j} R_i$$

$$T_j = \sum_{i=1}^{n} \omega_i^{\,j} I_i \qquad (4.3\text{-}38)$$

$$U_j = \sum_{i=1}^{n} \omega_i^{\,j}(I_i^{\,2}+R_i^{\,2})$$

The set of linear equations (4.3-37) can be expressed in matrix form as:

$$\underline{\underline{M}} \times \underline{N} = \underline{C} \qquad (4.3\text{-}39)$$

where

$$\underline{\underline{M}} = \begin{vmatrix} \lambda_0 & 0 & -\lambda_2 & 0 & \lambda_4 & \cdots & T_1 & S_2 & -T_3 & -S_4 & T_5 & \cdots \\ 0 & \lambda_2 & 0 & -\lambda_4 & 0 & \cdots & -S_2 & T_3 & S_4 & -T_5 & -S_6 & \cdots \\ \lambda_2 & 0 & -\lambda_4 & 0 & \lambda_6 & \cdots & T_3 & S_4 & -T_5 & -S_6 & T_7 & \cdots \\ 0 & \lambda_4 & 0 & -\lambda_6 & 0 & \cdots & -S_4 & T_5 & S_6 & -T_7 & -S_8 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots & \vdots & \vdots & \\ T_1 & -S_2 & -T_3 & S_4 & T_5 & \cdots & U_2 & 0 & -U_4 & 0 & U_6 & \cdots \\ S_2 & T_3 & -S_4 & -T_5 & S_6 & \cdots & 0 & U_4 & 0 & -U_6 & 0 & \cdots \\ T_3 & -S_4 & -T_5 & S_6 & T_7 & \cdots & U_4 & 0 & -U_6 & 0 & U_8 & \cdots \\ S_4 & T_5 & -S_6 & T_7 & S_8 & \cdots & 0 & U_6 & 0 & -U_8 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots & \vdots & \vdots & \end{vmatrix}$$

$$\underline{N} = \begin{vmatrix} b_0 \\ b_1 \\ b_2 \\ b_3 \\ \vdots \\ a_1 \\ a_2 \\ a_3 \\ a_4 \\ \vdots \end{vmatrix} \qquad \underline{C} = \begin{vmatrix} S_0 \\ T_1 \\ S_2 \\ T_3 \\ \vdots \\ 0 \\ U_2 \\ 0 \\ U_4 \\ \vdots \end{vmatrix}$$

The problem of evaluating the unknown coefficients in a transfer function is now reduced to the numerical solution of certain determinants.

d. Staffin and Staffin Technique

The procedure proposed by Staffin and Staffin (70) consists of matching the gain and phase angle curves or the gain curve only of the frequency response of a system by the transfer function described by equation (4.3-1a). First, it is necessary to group the odd and even powers of ω in equation (4.3-1b).

$$G(j\omega) = \frac{(b_m - b_{m-2}\omega^2 + \ldots) + j(b_{m-1}\omega - b_{m-3}\omega^3 + \ldots)}{(a_n - a_{n-2}\omega^2 + \ldots) + j(a_{n-1}\omega - a_{n-3}\omega^3 + \ldots)} \qquad (4.3\text{-}40a)$$

$$= \frac{N_e(\omega) + j\,N_0(\omega)}{D_e(\omega) + j\,D_0(\omega)} \qquad (4.3\text{-}40b)$$

where e and 0 refer to the terms in even and odd powers of ω respectively.

$G(j\omega)$ can be expressed as the sum of a real and an imaginary part as

$$G(j\omega) = R(\omega) + j\,I(\omega) \qquad (4.3\text{-}41)$$

For gain and phase matching, substitution of equation (4.3-41) into equation (4.3-40b) yields

$$N_e(\omega) + jN_0(\omega) = R(\omega)\,D_e(\omega) - I(\omega)\,D_0(\omega)$$

$$+ j[R(\omega)\,D_0(\omega) + I(\omega)\,D_e(\omega)] \qquad (4.3\text{-}42)$$

Equating the real and imaginary parts in equation (4.3-42) yields

$$N_e(\omega) = R(\omega)\, D_e(\omega) - I(\omega)\, D_0(\omega) \qquad (4.3\text{-}43a)$$

$$N_0(\omega) = R(\omega)\, D_0(\omega) + I(\omega)\, D_e(\omega) \qquad (4.3\text{-}43b)$$

If the frequency response data are given in terms of both the magnitude ratio and the phase angle, the real and imaginary parts of $G(j\omega)$ can be computed.

At a given frequency ω_i, it is possible to derive the following expressions using the definitions of N_e, N_0, D_e, D_0 from equations (4.3-40a) and (4.3-40b).

$$R_i(a_n - a_{n-2}\omega_i^2 + \ldots) - I_i(a_{n-1}\omega_i - a_{n-3}\omega_i^3 + \ldots)$$
$$= (b_m + b_{m-2}\omega_i^2 + \ldots) \qquad (4.3\text{-}44)$$

$$R_i(a_{n-1}\omega_i - a_{n-3}\omega_i^3 + \ldots) + I_i(a_n - a_{n-2}\omega_i^2 + \ldots)$$
$$= (b_{m-1}\omega_i + b_{m-3}\omega_i^3 + \ldots) \qquad (4.3\text{-}45)$$

where R_i and I_i are the real and imaginary parts of $G(j\omega_i)$ respectively.

In equations (4.3-44) and (4.3-45), there are $(n + 1)$ a_j and

(m+1) b_k unknowns, thus taking (n+m+2)/2 simultaneous equations which can be solved for the values of a_j and b_k.

For gain matching only, Staffin and Staffin recommended the following procedure.

Taking the magnitude of $G(j\omega)$ in equation (4.3-40b) yields

$$|G(j\omega)|^2 = \frac{[N_e(\omega)]^2 + [N_0(\omega)]^2}{[D_e(\omega)]^2 + [D_0(\omega)]^2} \qquad (4.3\text{-}46)$$

$|G(j\omega)|^2$ is a ratio of two polynomials of even powers of ω which can be written as:

$$|G(j\omega)|^2 = \frac{\beta_0+\beta_1\omega^2 +\ldots+\beta_m\omega^{2m}}{\alpha_0+\alpha_1\omega^2 +\ldots+\alpha_n\omega^{2n}} \qquad (4.3\text{-}47)$$

Values of α and β can be determined from $G(j\omega)$ by choosing (n+m+2) values of ω_i and solving the resulting simultaneous equations. Once the values of α and β are obtained, the values of a_j and b_k can be computed.

e. Rosenbrock Method in the Frequency-Domain

To demonstrate the usefulness of Rosenbrock's search technique, this method will be used to fit the transfer function of the form of equation (4.3-1a) to frequency response data.

To fit the amplitude ratio curve or the phase angle curve of the frequency response, it is necessary to derive an analytical expression of the magnitude ratio or the phase angle in function of the frequency.

At any specific frequency ω_i, the error between the model and the experimental data is:

$$e_i(\underline{p}) = y(\underline{p},\omega_i) - \phi(\omega_i) \tag{4.3-48}$$

where $y(\underline{p},\omega_i)$ is the value of the model calculated from the mathematical expression of the magnitude ratio or the phase angle at the frequency ω_i, $\underline{p}$ is the set of parameters to be determined and $\phi(\omega_i)$ is the experimental data at the frequency ω_i.

To curve fit the frequency response, it is proper to seek the least value of the equation:

$$F = \sum_{i=1}^{n} (y(\underline{p},\omega_i) - \phi(\omega_i))^2 \tag{4.3-49}$$

The minimum of the function F can now be obtained using the Rosenbrock search technique described in part A of section 4.3-2.

4.3.3 Criteria for Selecting the Simplest Adequate Representation

In all the methods of determining the approximate transfer function considered so far, either the degree of the numerator and the denominator of equation (4.3-1a) (m and n) or the form of the transfer function (first, second or third order) must be estimated.

If the equation (4.3-1a) was chosen to fit the experimental data, it is preferable to start with small values of m and n. In the case where the match is not satisfactory, the estimated values of m

and n must be increased until a satisfactory match is obtained. If the values of m and n chosen were too high, some poles and zeros found by curve fitting are far from the other poles and zeros so they are considered to be spurious and can normally be dropped.

Since in practice, most systems can be adequately represented by a first, a second or a third order transfer function, the problem then arises is as how to select the simplest transfer function which still can adequately represent the dynamics of the system. Bailey and Law (8) proposed a simple method which can be used as an answer to this problem. The method will be outlined as follows.

Assuming that any errors in the data are insignificant when compared to the errors due to lack of fit between the model and the data. The residual sum of squares is a measure of the errors due to lack of fit. The sum of squares for assumed first, second and third order systems are given by the following equations:

$$S_1^2 = \sum_{i=1}^{n} (y_{1i}-\phi_i)^2 \tag{4.3-50}$$

$$S_2^2 = \sum_{i=1}^{n} (y_{2i}-\phi_i)^2 \tag{4.3-51}$$

$$S_3^2 = \sum_{i=1}^{n} (y_{3i}-\phi_i)^2 \tag{4.3-52}$$

where y_{1i} = model for first order system representation

y_{2i} = model for second order system representation

y_{3i} = model for third order system representation

S_1^2 = residual sum of squares for first order system representation

S_2^2 = residual sum of squares for second order system representation

S_3^2 = residual sum of squares for third order system representation

ϕ_i = experimental data

Bailey and Law then selected the model on the basis of a statistical test performed on S_1^2, S_2^2 and S_3^2 .

Since all residual sums of squares are calculated from the same number of data points, the ratios $[S_1^2/S_3^2]$ and $[S_2^2/S_3^2]$ will be distributed as the F distribution with (n-1,n-3) and (n-2,n-3) degrees of freedom (n is the total number of data points). The following criteria were used to select the simplest adequate representation:

(i) If $[S_2^2/S_3^2] \geq F_{1-\alpha}(n-2,n-3)$: use third order system representation

(ii) If $[S_2^2/S_3^2] < F_{1-\alpha}(n-2,n-3)$: make the following test:

- If $[S_1^2/S_3^2] \geq F_{1-\alpha}(n-1,n-3)$: use second order system representation
- If $[S_1^2/S_3^2] < F_{1-\alpha}(n-1,n-3)$: use first order system representation

where α is the level of significance of the F distribution (α was taken as equal to 0.01 by Bailey and Law).

For a detailed discussion of the statistical reasoning in-

volved in the above criteria, reference (18) should be consulted.

Although this method was used originally by Bailey and Law to find the simplest adequate representation of frequency response data, it has also been used in this study to select the simplest transfer function representation of time-domain data.

4.4 Illustrative Examples Used to Evaluate the Different Methods of Determining Approximate Transfer Functions

To compare various methods of determining approximate system transfer functions, computations were carried out using data from two known second order transfer functions.

The transfer functions selected were:

Example 1

$$G(s) = \frac{5.0}{(9.0s+1)(10.0s+1)}$$

Example 2

$$G(s) = \frac{5.0}{(0.5s+1)(10.0s+1)}$$

To obtain the data used for curve fitting, the time-domain data were generated from the analytical expressionsas given by the above transfer functions to a rectangular pulse forcing function of known magnitude and duration.

The frequency response data were obtained by computing the

Table 4.4-1

Determination of the Transfer Functions by Different Methods for Example 1

	A*	B*	C*	D*	E*	F*	G*
K	5.000	5.024	5.000	4.882	4.991	5.000	5.000
τ_1	9.000	9.282	9.096	8.921	8.963	9.120	9.423
τ_2	10.000	10.271	9.898	9.531	10.043	9.980	9.573

Table 4.4-2

Determination of the Transfer Functions by Different Methods for Example 2

	A*	B*	C*	D*	E*	F*	G*
K	5.000	5.007	5.000	4.975	5.000	5.000	5.000
τ_1	0.500	0.478	0.501	0.623	0.500	0.502	0.500
τ_2	10.000	10.528	9.999	9.825	10.000	9.988	9.988

*Column A lists the original transfer function coefficients, and columns B,C,D,E,F,G denote the parameters of the transfer function determined by the Rosenbrock method in the time-domain and the methods of Bailey and Law; Chen and Philip; Levy; Staffin and Staffin and of Rosenbrock in the frequency-domain respectively.

magnitude ratios and the phase angles at various frequencies using their known mathematical expressions corresponding to the above transfer functions.

Table 4.4-1 summarizes the parameters of the transfer function in Example 1 determined by different methods and Table 4.4-2 contains the results for Example 2.

4.5 Discussion

Results from using the different methods of determining an approximate transfer function revealed the following points:

(i) Rosenbrock method ÷ One of the difficulties with the Rosenbrock search technique is the lack of a satisfactory criterion to terminate the search. Indeed, as the case with any hill-climbing method, it is difficult to know when the optimum is reached. Rosenbrock suggested that it is preferable to stop the search after a predetermined number of steps, and a rough estimation is that about $50 \times \ell$ evaluations of the function $F(\underline{p})$ to be optimized will often suffice (ℓ is the number of parameters to be determined). This might lead to inefficiency in simple problems where only a small number of iterations is required to find the desired solution. For some particular problems, this estimated number of $50 \times \ell$ is not enough since progress to the optimum may be slow and furthermore the optimum values may not have been established. For these difficult problems, it is desirable to print out all the step lengths d_i, the direction $\underline{v}_i$, and the values of the function $F(\underline{p})$. If inspection shows that a minimum has not been reached,

re-start the search using as initial approximations of the variables $\underline{p}$, the best values of the parameters determined by the previous research.

In general, when a very large number of data points is involved, the evaluation of the function $F(\underline{p})$ is relatively slow. The computer time will then depend much less on the search technique and much more on the number of evaluations of $F(\underline{p})$.

(ii) Bailey and Law method ÷ With this method, it is possible to curve fit the transfer function using only amplitude ratio data. This is particularly desirable since phase angle experimental data are unreliable at high frequencies. The requirement of the partial derivatives of the function to be optimized would limit this method, for all practical purposes, to simple transfer functions only. The Bailey and Law technique gives fast convergence, but sometimes, it might lead to undesirable solutions of the parameters to be determined.

(iii) Chen and Philip method ÷ This method has the advantages of eliminating an early decision as to the form of the transfer function and the procedure is easily programmed on a digital computer. However, determination of an approximate transfer function by this method is impracticable since:

- To evaluate the Fourier coefficients A_k in equation (4.3-28), the data of $R(\theta)$ should be available for the interval $\theta(0,2\pi)$ for the variable θ would correspond to the interval $(0,\infty)$ for the frequency variable ω. In practice, it is a known fact that frequency response data, especially phase angle data are not available, or highly unreliable.

- For transfer functions of complicated forms, a very large number of Fourier coefficients A_k would need to be evaluated since there is not a sharp drop-off in the values of A_k. The conversion from the variables A_k in equation (4.3-25) to the transfer function coefficients a_j and b_k in equation (4.3-1a) might be a troublesome problem.

(iv) Levy method ÷ The most desirable feature of the Levy technique is that it can be used to fit transfer functions of any form (the degree of the numerator m and denominator n in equation (4.3-1a) need to be specified) without making any modification in the computer program. The only restriction is that this method is confined to systems having a finite magnitude at zero frequency. For the determination of parameters in simple transfer functions, Levy's method is somewhat inferior to Bailey and Law's method because it requires phase angle experimental data, and furthermore, it gives more emphasis in the curve fitting scheme to data at high frequencies, which might lead to serious errors since frequency response data are generally least reliable at high frequencies.

(v) Staffin and Staffin method ÷ Since only a very limited number of data points can be utilized to determine the transfer function coefficients, it is suggested that the data be taken at some previously set increment of frequency or completely at random to avoid bias in the selection of data points. This method has certain deficiencies regarding accuracy and general applicability since there is no allowance for measurement error.

(vi) Determination of an approximate transfer function from time-domain data versus frequency-domain data ÷ It might appear from the results given by Tables 4.4-1 and 4.4-2 that the determination of the transfer function from frequency response data particularly by the methods of Levy (37) and Bailey and Law (8) gives a better approximation of the true transfer function coefficients than the determination of the transfer function coefficients from time-domain data by Rosenbrock's search technique. It seems likely that this is due to the fact that in application of Rosenbrock's method in the time-domain, the initial approximations of the parameters $\underline{p}$ were chosen to be far away from the correct values of $\underline{p}$ and the convergence toward the absolute minimum of $F(\underline{p})$ in equation (4.3-6) is relatively slow.

It should be remembered however, that in practice it is often desirable to determine the transfer function directly from time-domain data because if frequency response data are generated from time-domain data through data reduction techniques, which is the case of pulse testing, possible errors would result in the frequency response data. Furthermore, a "best" fit in the frequency-domain does not necessarily yield a "best" fit in the time-domain.

CHAPTER V

DISTILLATION COLUMN DYNAMICS

5.1 Introduction

Knowledge of the dynamic behavior of a process is the first step in the development of improved control schemes. A rigorous mathematical model of the distillation column although possible, is not of value for practical purposes because even the use of approximate models involves the solution of a large number of differential equations. The computational time may also be prohibitive for practical utility. For control purposes, at least when conventional three-mode controllers are considered, only a simple representation which adequately describes the dynamic characteristics of the column is needed.

It is common practice, in process control, to develop a set of transfer functions which are able to approximate as close as possible to the actual process responses. Such an approach can be extremely rewarding as long as the perturbations being considered are small compared with the average values of the associated independent variables.

This chapter summarizes some of the literature concerned with dynamic models of distillation columns and is concluded with the models used in this study. Models were developed from the experimental transient responses of two pilot-scale distillation columns: one from the University of Delaware and the other from the University of Alberta, by

assuming that the dynamic responses of these two columns can be represented by first or second order plus time delay transfer functions, i.e.

$$G(s) = \frac{Ke^{-\tau_D s}}{(\tau_1 s+1)} \qquad (5.1\text{-}1)$$

or

$$G(s) = \frac{Ke^{-\tau_D s}}{(\tau_1 s+1)(\tau_2 s+1)} \qquad (5.1\text{-}2)$$

5.2 Literature Survey on Distillation Column Dynamics

Considerable information has appeared in the recent literature concerning the dynamic behavior of distillation columns. For the simplest cases, along with many restricting assumptions, the resulting differential equations describing the transient responses of distillation columns can be solved analytically (47,78). With the increased availability of analog and digital computers, it has become possible to solve more sophisticated models, however, in some cases, severe assumptions on the models proposed. This is particularly true, in the cases where analog computers have been used; linearization of the mathematical models is employed in order to ease the very high requirement for non-linear components on analog computers (40,60,79,80). Recently, solutions of the dynamic models of distillation columns have been carried out on digital computers for both binary (61,73) and multicomponent cases (31,62). Very complete surveys which cover most of the

aspects of distillation column dynamics can be found in the literature (31,73,83). Especially noteworthy is a comprehensive review by Williams (83) which summarized the guidelines to be used in formulating a mathematical model for a plate distillation column along with many common simplifying assumptions used to reduce the enormous complexity of the original equations.

Instead of theoretical models, empirical models in the form of low order transfer functions have been proposed by several authors (30,32,58,85). Hoyt and Stanton (32) have shown that the response of the liquid temperature on an intermediate tray to boil-up rate change or feed rate change can be approximated by a first order plus time delay model. This type of model has been used by Pacey (52) to represent the responses of top and bottom product compositions for feed flow rate and reflux flow rate variations. A second order plus time delay model transfer function has been suggested by Rees (58). It was found that the accuracy of this model is better than 3 per cent for small perturbations around the steady-state operating point. First, second and higher order transfer functions have been used by Moczek et al (49). They proved by illustrative examples that the parameters of the transfer functions exhibited a strong dependence upon the magnitude and direction of a particular upset, due to the non-linear behavior of the column. This observation was also confirmed by Pacey (52), Rees (58) and Bornard et al (15).

Studies dealing with experimental testing of distillation

columns to determine the overall transfer functions describing the column dynamics originally utilized transient and frequency response techniques. However, during the past few years, most studies have concentrated on use of pulse testing method (46,52), since pulses are in general easy to produce and exact pulse shapes are not critical. Furthermore, the system is upset only for a very short period and then returns to its original conditions. Pulse testing often reveals information about the system at frequencies which are unobtainable by direct frequency response techniques. Marino and Stutzman (46) showed that the pulse testing technique, with a rectangular pulse, in general gives good agreement with results from direct frequency response testing provided that optimum pulse widths are used.

5.3 Dynamic Models of the University of Delaware Distillation Column

Extensive experimental studies have been carried out on a ten-tray, two-foot diameter, bubble cap distillation column at the University of Delaware by Gerster and co-workers (40,42,69). The column was operated with the acetone-benzene system with feed entering the column as a liquid on the 5th tray up from the bottom. A complete description of the column along with all pertinent data are given in reference (40). Although the column contained ten intermediate trays, only the composition of the liquid on trays 1, 3, 5, 7, 9 was measured during the transient periods.

Experimental data from runs Nos. 8, 6-V and 10-V (run designation used by Gerster el al (40)) were used in deriving the models used

Table 5.3-1

Parameters for the Models of the University of Delaware Distillation Column for Feed Composition Changes

	τ_D(min.)	K($\frac{\text{mole \%}}{\text{mole \%}}$)	τ_1(min.)	τ_2(min.)
Top composition	2.0	0.9	5.5	6.0
Tray 9*	-	1.8	6.5	-
Tray 7*	-	2.5	5.4	-
Tray 3*	-	3.5	0.1	5.0
Tray 1*	-	2.9	0.5	8.0
Bottom composition	-	2.5	3.0	7.0

*Parameters are for the transfer function relating the liquid composition on an intermediate tray to feed composition changes.

Table 5.3-2

Parameters for the Models of the University of Delaware Distillation Column for Reflux Flow Rate Changes

	τ_D(min.)	$K(\frac{\text{mole \% x min.}}{\text{lb. mole}})$	τ_1(min.)	τ_2(min.)
Top composition	1.0	29.5	3.5	5.3
Tray 9*	-	59.8	5.9	-
Tray 7*	-	90.9	6.4	-
Tray 3*	0.5	101.5	7.4	-
Tray 1*	1.0	83.3	10.3	-
Bottom composition	1.0	31.8	5.5	6.5

*Parameters are for the transfer function relating the liquid composition on an intermediate tray for reflux flow rate changes.

Table 5.3-3

Parameters for the Models of the University of Delaware Distillation Column for Boil-up Rate Changes

	τ_D(min.)	$K(\frac{\text{mole \% x min.}}{\text{lb. mole}})$	τ_1(min.)	τ_2(min.)
Top composition	2.0	-34.8	1.5	11.0
Tray 9*	-	-72.1	12.5	-
Tray 7*	-	-77.2	11.0	-
Tray 3*	-	-83.7	1.0	10.0
Tray 1*	-	-96.2	1.5	9.0
Bottom composition	-	-46.2	2.0	8.0

*Parameters are for the transfer function relating the liquid composition on an intermediate tray for boil-up rate changes.

in this study due to the following reasons:

(i) Initial steady-state conditions for these runs were nearly the same. These operating conditions are listed in Appendix A.1.

(ii) Sizes of input disturbances were relatively small, so the system can be regarded as approximately linear.

The models utilized were established by adjusting different values of the parameters in equations (5.1-1) or (5.1-2) until there was a good fit between the models and experimental data. The goodness of fit was judged simply by visual observation.

Tables 5.3-1, 5.3-2 and 5.3-3 list the empirical models established from the data obtained by Gerster and co-workers and used in this study to describe the composition dynamics of the column for changes in feed composition, reflux flow rate and boil-up rate respectively.

5.4 Dynamic Models of the University of Alberta Distillation Column

A description of the University of Alberta distillation column can be found in Chapter VII. Process transfer functions of this column for different types of disturbances such as feed flow rate, reflux flow rate and steam flow rate have been determined using pulse testing data taken by Berry and Pacey (13). For each disturbance, rectangular pulses of different magnitudes and directions were introduced into the column. The initial steady-state operating conditions were maintained nearly constant during all tests. A typical list of steady-state data is given in Table 5.4-1.

Table 5.4-1

Typical Steady-State Conditions of the

University of Alberta Distillation Column

Feed flow rate	2.589 lb./min.
Reflux flow rate	2.196 lb./min.
Steam flow rate	1.973 lb./min.
Top product flow rate	1.331 lb./min.
Bottom product flow rate	1.299 lb./min.
Feed composition	46.00 weight % methanol
Top product composition	95.89 weight % methanol
Bottom product composition	0.60 weight % methanol
Temperature of the liquid on tray 1	206.1°F
Temperature of the liquid on tray 2	197.5°F
Temperature of the liquid on tray 3	182.6°F
Temperature of the liquid on tray 4	173.5°F
Temperature of the liquid on tray 5	163.9°F
Temperature of the liquid on tray 6	157.0°F
Temperature of the liquid on tray 7	152.2°F
Temperature of the liquid on tray 8	148.8°F
Pressure in the condenser	-0.1 in. of H_2O
Feed temperature	163.4°F
Reflux temperature	150.0°F

The necessary data for determining the transfer functions namely, the disturbance flow rate, the top product composition, the bottom product composition and the liquid temperature on intermediate trays in addition to values of other variables were collected using the data acquisition capability of the real-time IBM 1800 digital computer. Off-line identification of process parameters for models of the form given by equations 5.1-1 or 5.1-2 was done using the Oldenbourg and Sartorius' method (50) to calculate the time delays and Rosenbrock's search procedure (63) to determine the best values of gains, time constants by fitting experimental data in the time-domain. Finally, Bailey and Law's criteria (8) was used for selecting the simplest form of transfer function.

It was found that the data from all tests could be adequately represented by second order plus time delay transfer functions. Furthermore, all the parameters exhibited some dependence upon the particular test so average values of these parameters were employed. The parameters of the models used in this study are given in Tables 5.4-2, 5.4-3 and 5.4-4. The pulse testing data are given in the distillation column data book (13).

Table 5.4-2

Parameters for the Models of the University of Alberta Distillation Column for Feed Flow Rate Changes

	τ_D(min.)	K	τ_1(min.)	τ_2(min.)
Top composition	3.5	6.5	5.1	18.2
Tray 8*	3.5	- 4.1	4.3	13.3
Tray 7*	3.2	- 7.4	6.0	12.3
Tray 6*	1.6	-15.1	4.3	14.2
Tray 5*	1.1	-22.6	2.7	14.2
Tray 4*	-	-23.9	0.6	14.7
Tray 3*	-	-39.8	0.6	14.3
Tray 2*	0.5	-42.1	0.5	13.4
Tray 1*	1.1	-25.0	0.6	11.9
Bottom composition	3.6	3.7	0.6	12.9

*Parameters are for the transfer function relating the liquid temperature on an intermediate tray to feed flow rate changes

Table 5.4-3

Parameters for the Models of the University of Alberta Distillation Column for Reflux Flow Rate Changes

	τ_D(min.)	K	τ_1(min.)	τ_2(min.)
Top composition	-	19.7	0.5	27.7
Tray 8*	-	-10.8	0.4	20.6
Tray 7*	0.3	-20.6	0.4	20.0
Tray 6*	0.5	-35.2	0.6	20.7
Tray 5*	0.8	-45.2	0.8	19.6
Tray 4*	1.1	-42.2	1.3	17.6
Tray 3*	1.3	-69.7	1.5	19.0
Tray 2*	1.6	-71.6	1.9	18.2
Tray 1*	1.9	-32.8	1.9	12.5
Bottom composition	4.5	4.9	2.7	13.7

*Parameters are for the transfer function relating the liquid temperature on an intermediate tray to reflux flow rate changes.

Table 5.4-4

Parameters for the Models of the University of Alberta Distillation Column for Steam Flow Rate Changes

	τ_D(min.)	K	τ_1(min.)	τ_2(min.)
Top composition	1.1	-24.8	4.1	16.0
Tray 8*	-	20.3	3.2	16.4
Tray 7*	-	36.1	2.7	15.8
Tray 6*	-	58.8	2.2	16.1
Tray 5*	-	84.9	1.3	16.6
Tray 4*	-	81.9	0.4	16.4
Tray 3*	-	134.5	0.6	16.2
Tray 2*	-	149.2	0.6	15.9
Tray 1*	-	93.4	0.8	15.6
Bottom composition	3.3	-14.0	2.1	14.2

*Parameters are for the transfer function relating the liquid temperature on an intermediate tray to steam flow rate changes.

For Tables 5.4-2, 5.4-3 and 5.4-4, the following units apply:

(i) For top and bottom product composition changes,

$$K: \frac{\text{weight \% x min.}}{\text{lb.}}$$

(ii) For the liquid temperature on an intermediate tray changes,

$$K: \frac{{}^\circ\text{F x min.}}{\text{lb.}}$$

CHAPTER VI

SIMULATION

6.1 Introduction

The most common approach to predict the time response of a process is to simulate the system on an analog or a digital computer. As analog computers are generally limited in the number of computing elements they contain and by the accuracy of these elements, the simulation of large or complicated systems, especially those with time delays, is more convenient if done on a digital computer. In recent years, many digital simulation languages have become available to facilitate the simulation of systems using the digital computer. One of these languages, S/360 CSMP (System/360 Continuous System Modeling Program) has been implemented on the IBM 360 computer in the Computing Center of the University of Alberta. It is a simulation-oriented program designed to accept problems expressed in the form of a block diagram or a system of ordinary differential equations. The program includes a basic set of functional blocks with which the components of a continuous system may be presented, and accepts application oriented statements for defining the connection between these functional blocks. S/360 CSMP also accepts FORTRAN statements. Data input and output are facilitated by means of application-oriented control statements. Detailed information is available in the appropriate manuals (33,34).

6.2 Definition of the Problem

The objective of the present simulation study is to predict the control performance of a distillation column when either the top product composition or the bottom product composition or the composition (or temperature) on one of the intermediate trays is to be maintained constant in spite of external disturbances, and to determine from the control behavior of the process, which tray is the most suitable to control the top or bottom product composition when either the reflux or the steam flow is used as the corrective variable. As most distillation control systems are regulatory in nature, the function of the system is to hold the controlled variable steady at the value set by the reference despite any disturbance imposed externally, the optimum controller settings will be based upon a step change in either the feed composition or the feed flow rather than a change in the set point. This can be done by defining a performance function. The selection of such a function to evaluate the transient behavior of closed loop systems is arbitrary since no single, all encompassing "optimum performance criterion" exists. Since large initial errors in the transient responses are to be avoided, the optimum controller constants are taken as those that minimize the penalty function $\int_0^\infty e^2\,dt$ (integral of the squared error - I.S.E.).

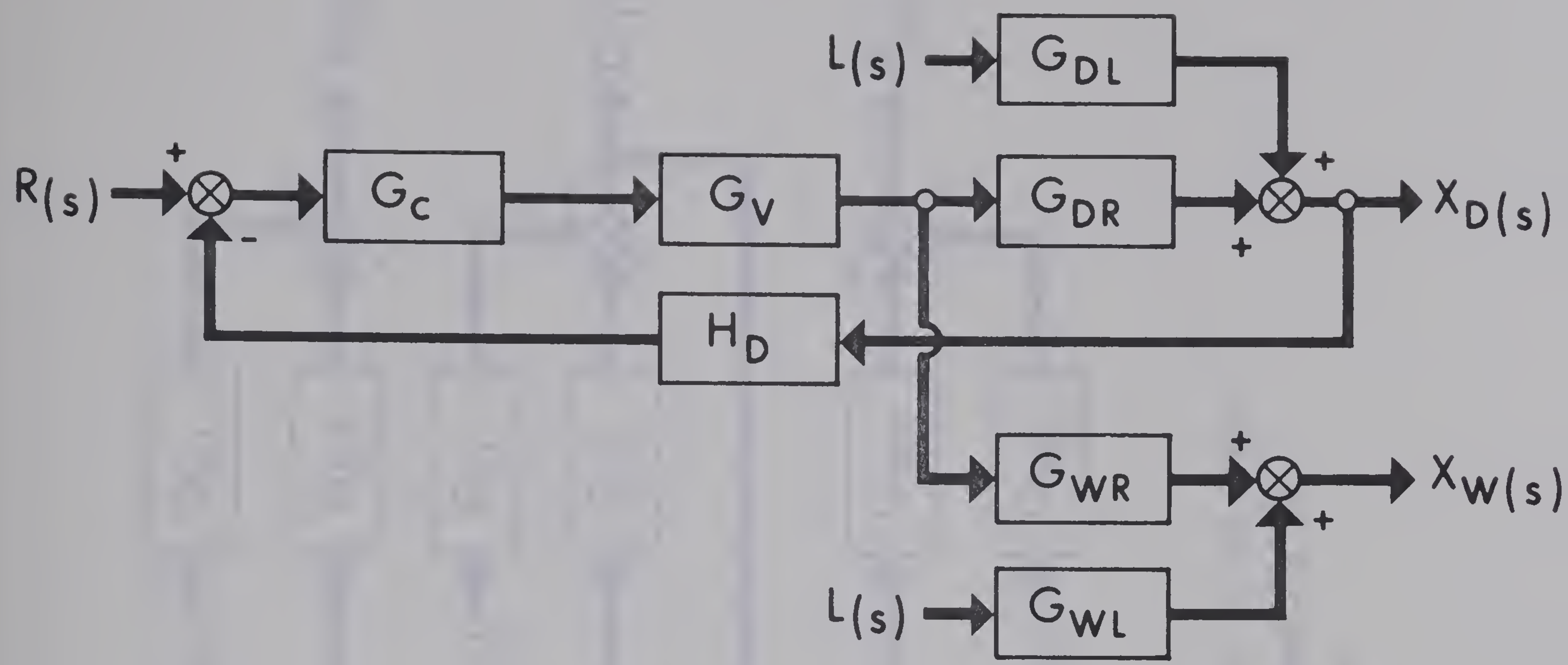


Figure 6.3-1 Block Diagram of Feedback Control of Top Product Composition by Manipulation of Reflux Flow

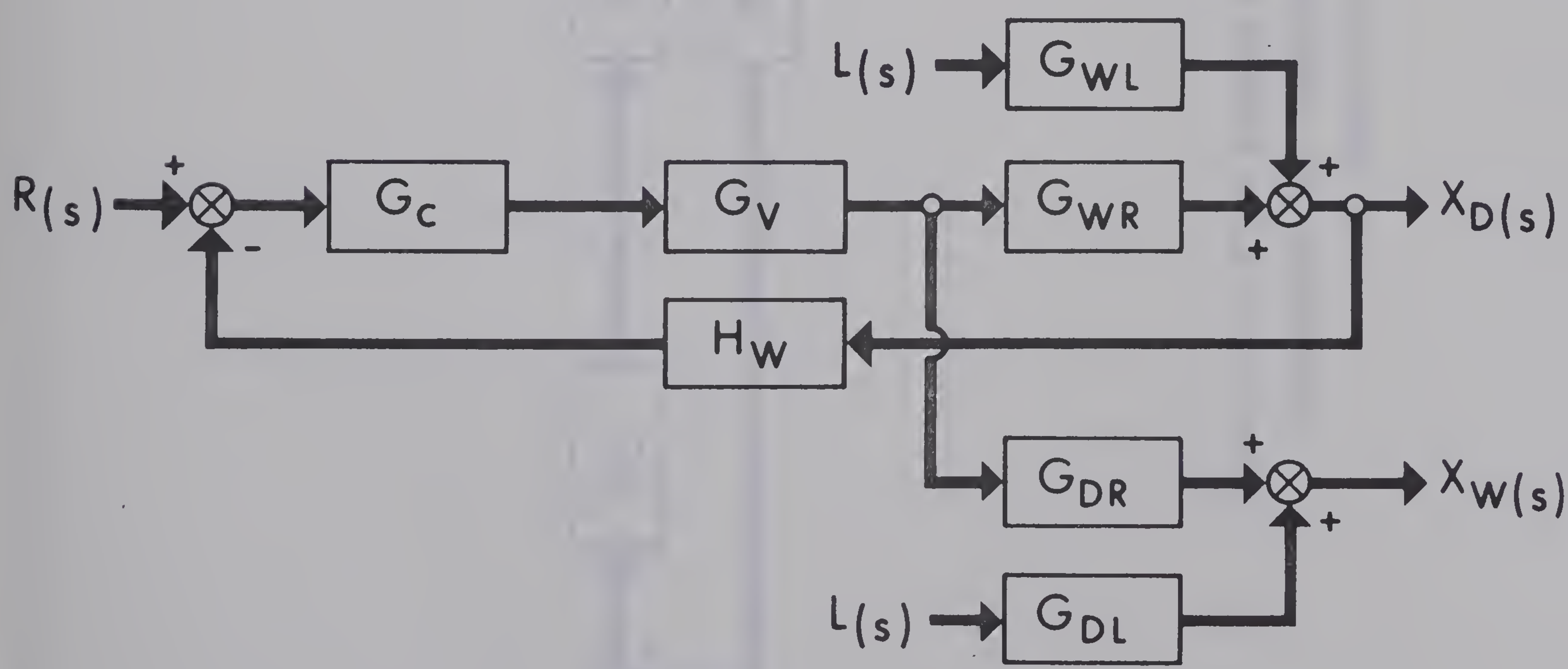


Figure 6.3-2 Block Diagram of Feedback Control of Bottom Product Composition by Manipulation of Reflux Flow

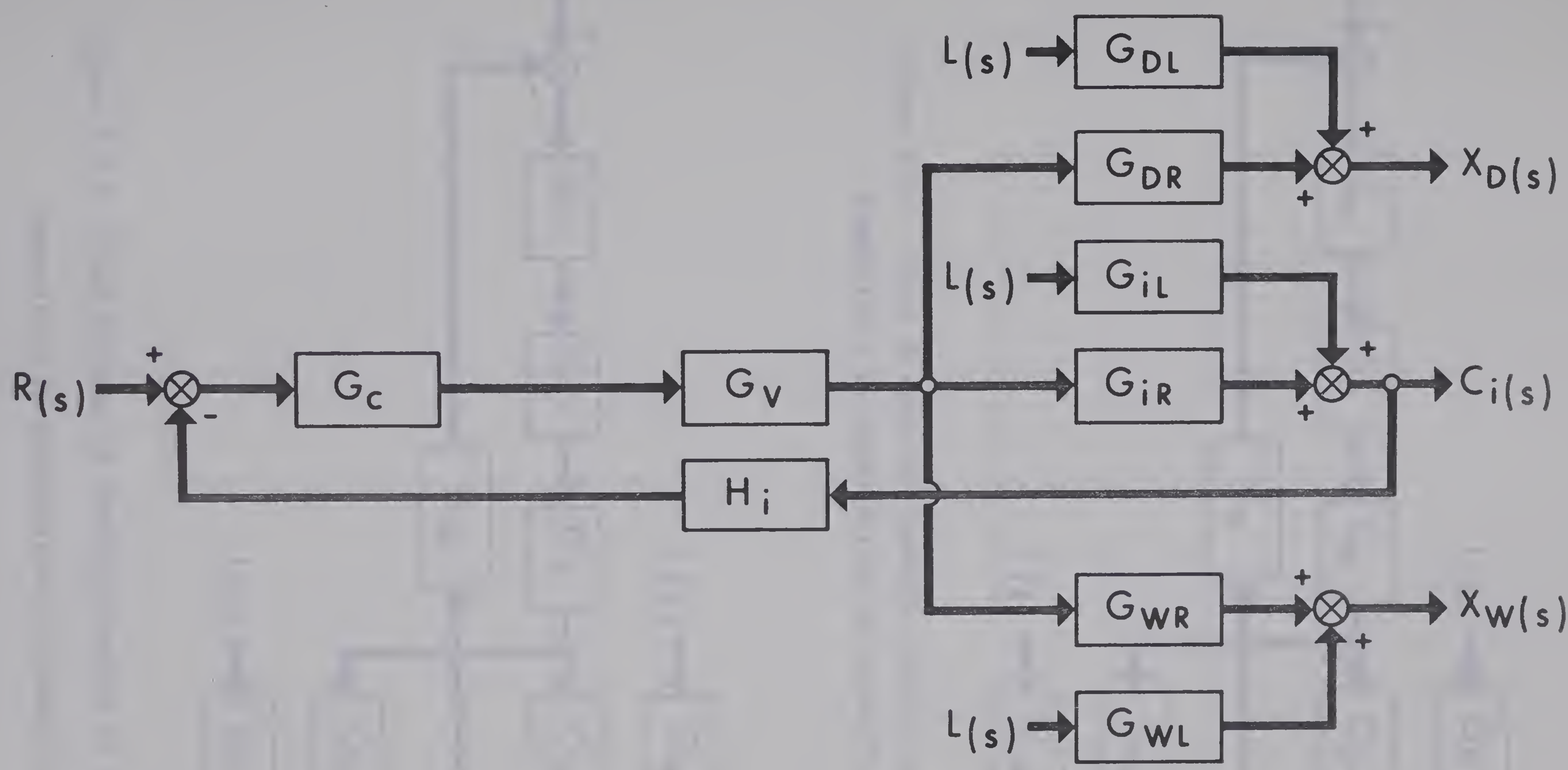


Figure 6.3-3 Block Diagram of Feedback Control of the Liquid Temperature (or Composition) on an Intermediate Tray by Manipulation of Reflux Flow

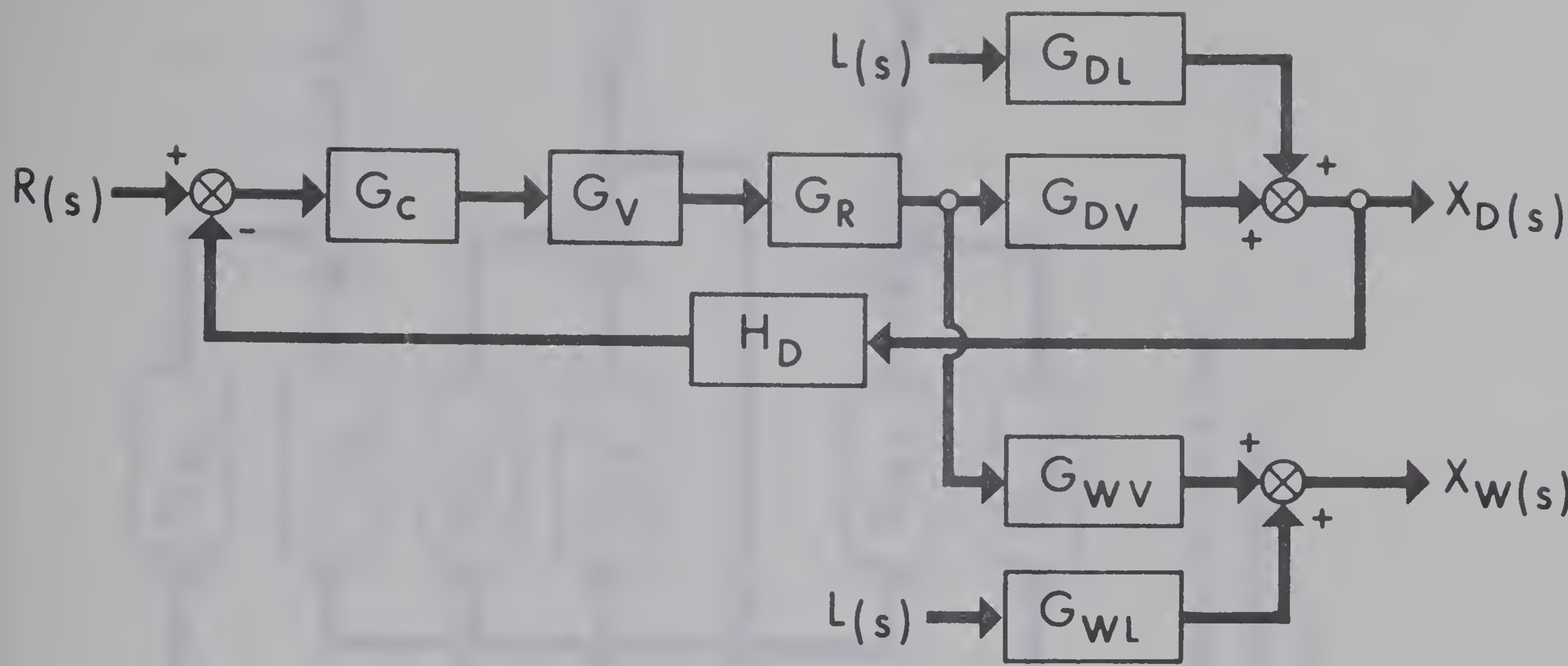


Figure 6.3-4 Block Diagram of Feedback Control of Top Product Composition by Manipulation of Steam Flow

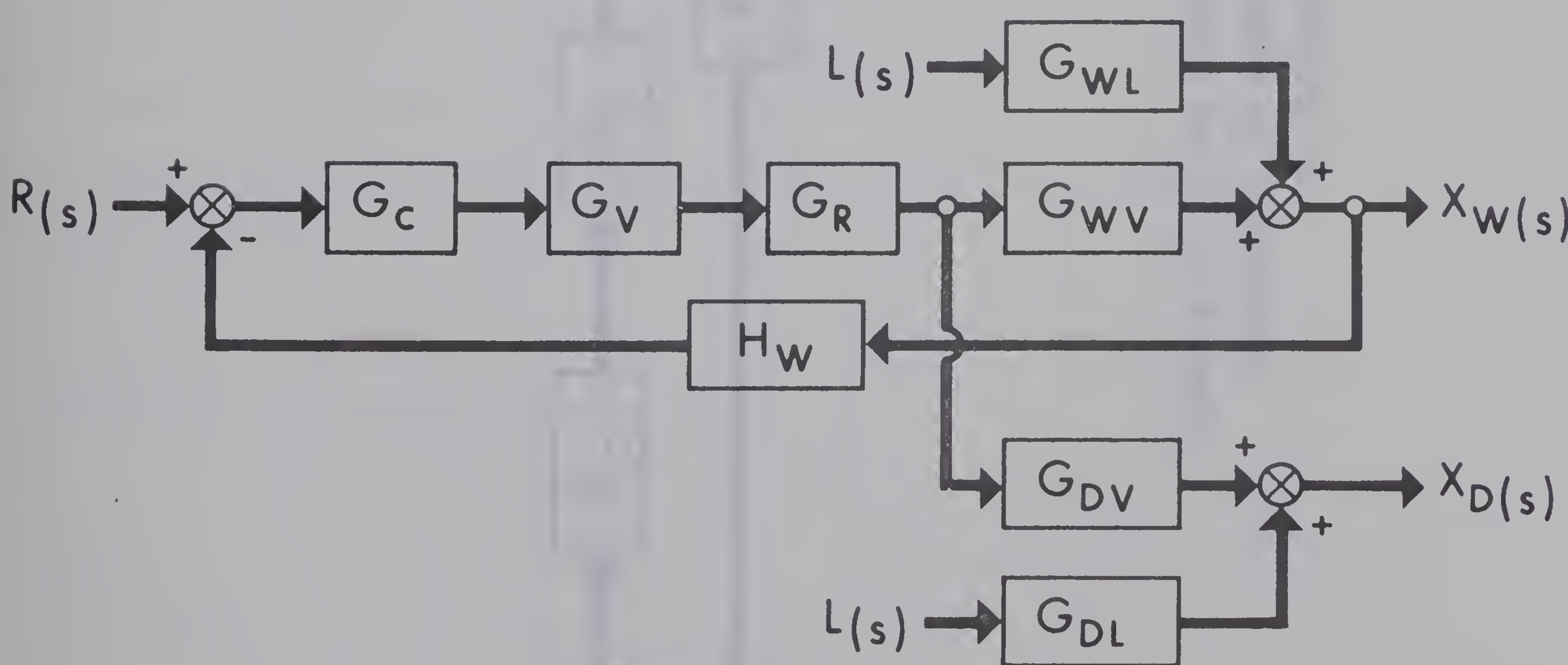


Figure 6.3-5 Block Diagram of Feedback Control of Bottom Product Composition by Manipulation of Steam Flow

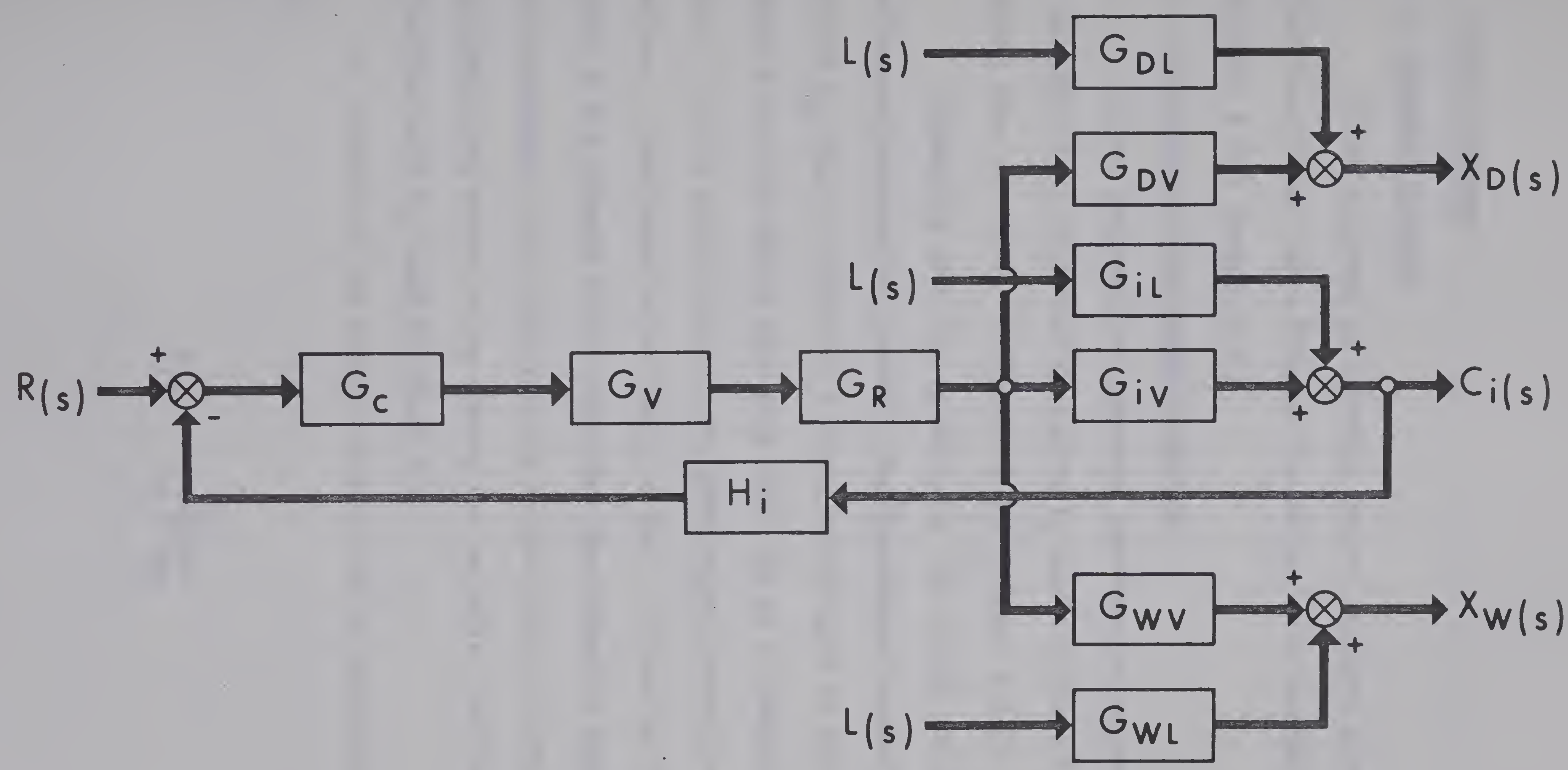


Figure 6.3-6 Block Diagram of Feedback Control of the Liquid Temperature (or Composition) on an Intermediate Tray by Manipulation of Steam Flow

6.3 Block Diagrams

6.3.1 Feedback Control

Block diagrams of feedback control schemes using either the reflux flow or the steam flow as the manipulative variable are shown in Figures 6.3-1 through 6.3-6.

6.3.2 Feedforward Plus Feedback Control

Block diagrams for combined feedforward-feedback systems for controlling a distillation column by manipulation of reflux flow or steam flow are shown in Figures 6.3-7 through 6.3-12.

Depending upon the dynamics of the column and the type of feedforward compensation desired, the feedforward controller transfer function G_{FF} may be simple as a proportional gain or have a form such as gain plus time delay, gain plus time lag or a combination of both types. For the present study, the feedforward controller transfer function is considered to be simply a gain. It can be shown from Figures 6.3-7 through 6.3-12 that when the column is subjected to a load disturbance, with feedforward control only, if there is to be no steady-state error in the controlled variable, the feedforward controller gain K_{FF} must be equal to:

(i) Control of top product composition by manipulation of reflux flow

$$K_{FF} = - \frac{K_{DL}}{K_V \times K_{DR}} \tag{6.3-1}$$

(ii) Control of bottom product composition by manipulation of reflux flow.

$$K_{FF} = - \frac{K_{WL}}{K_V \times K_{WR}} \tag{6.3-2}$$

(iii) Control of the composition (or temperature) of the liquid on intermediate tray i by manipulation of reflux flow.

$$K_{FF} = - \frac{K_{iL}}{K_V \times K_{iR}} \tag{6.3-3}$$

(iv) Control of top product composition by manipulation of reboil vapor rate.

$$K_{FF} = - \frac{K_{DL}}{K_V \times K_R \times K_{DV}} \tag{6.3-4}$$

(v) Control of bottom product composition by manipulation of re-boil vapor rate.

$$K_{FF} = - \frac{K_{WL}}{K_V \times K_R \times K_{WV}} \tag{6.3-5}$$

(vi) Control of the composition (or temperature) of the liquid on intermediate tray i by manipulation of reboil vapor rate.

$$K_{FF} = - \frac{K_{iL}}{K_V \times K_R \times K_{iV}} \tag{6.3-6}$$

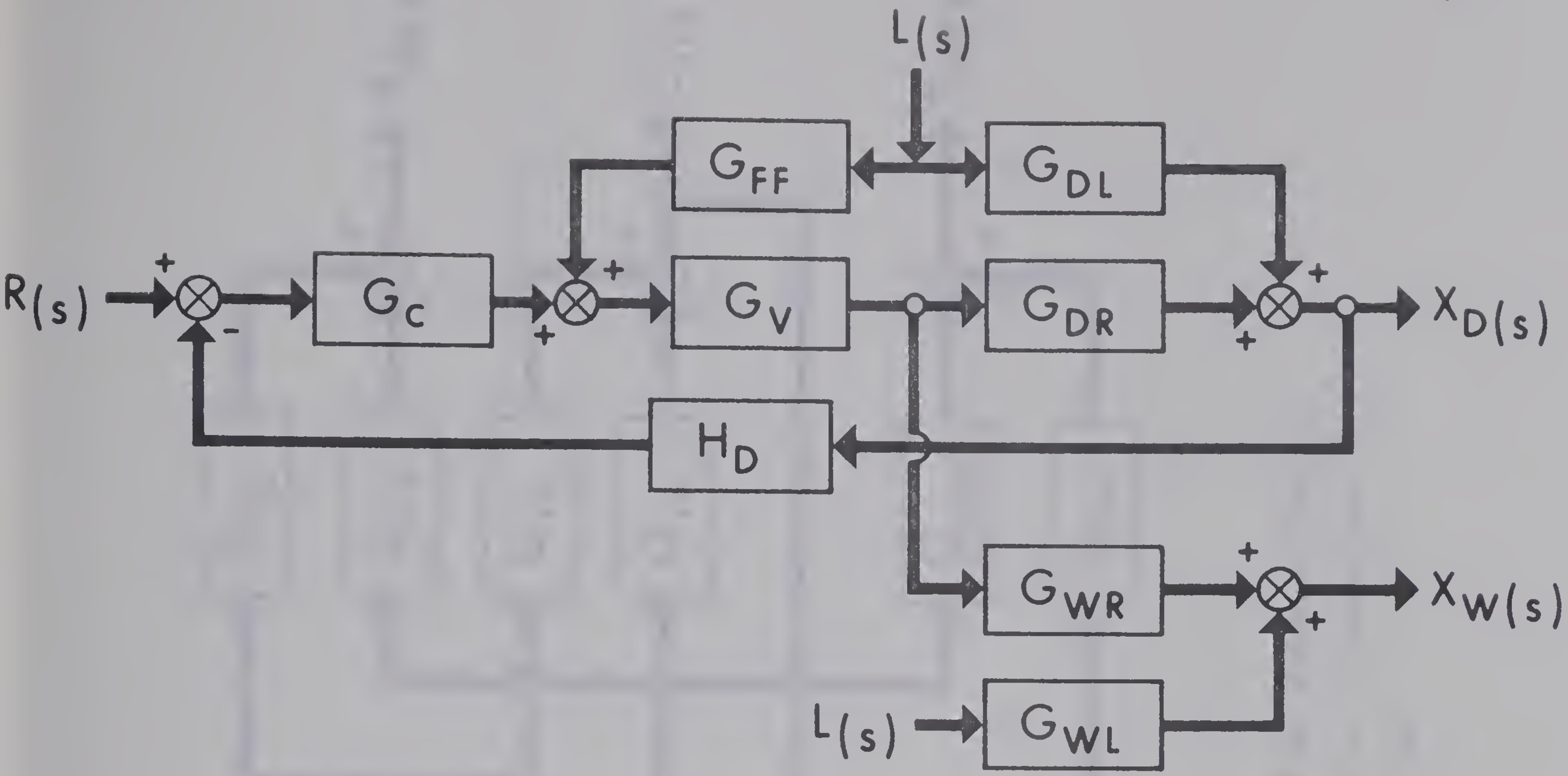


Figure 6.3-7 Block Diagram of Feedforward Plus Feedback Cotnrol of Top Product Composition by Manipulation of Reflux Flow

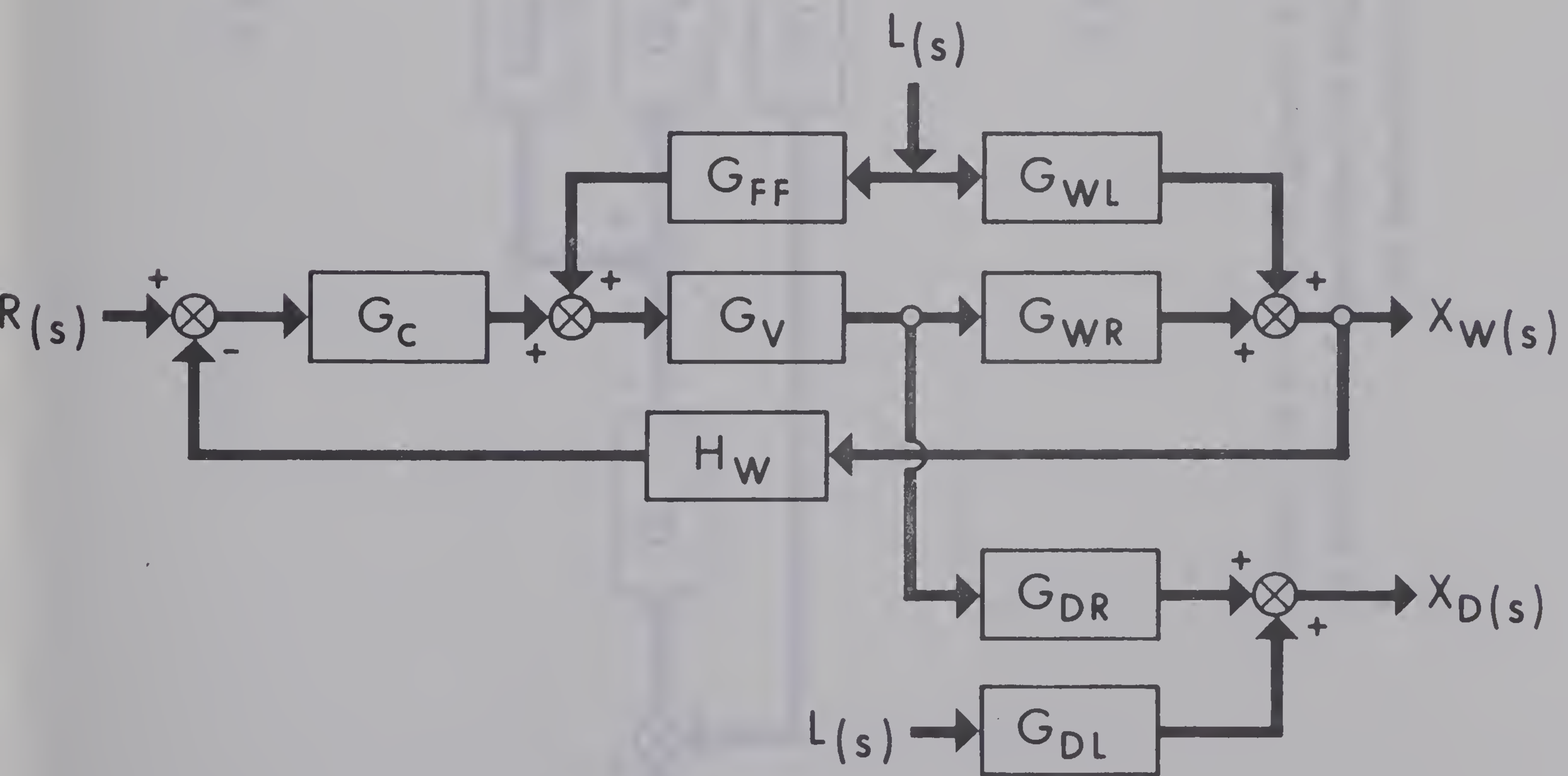


Figure 6.3-8 Block Diagram of Feedforward Plus Feedback Control of Bottom Product Composition by Manipulation of Reflux Flow

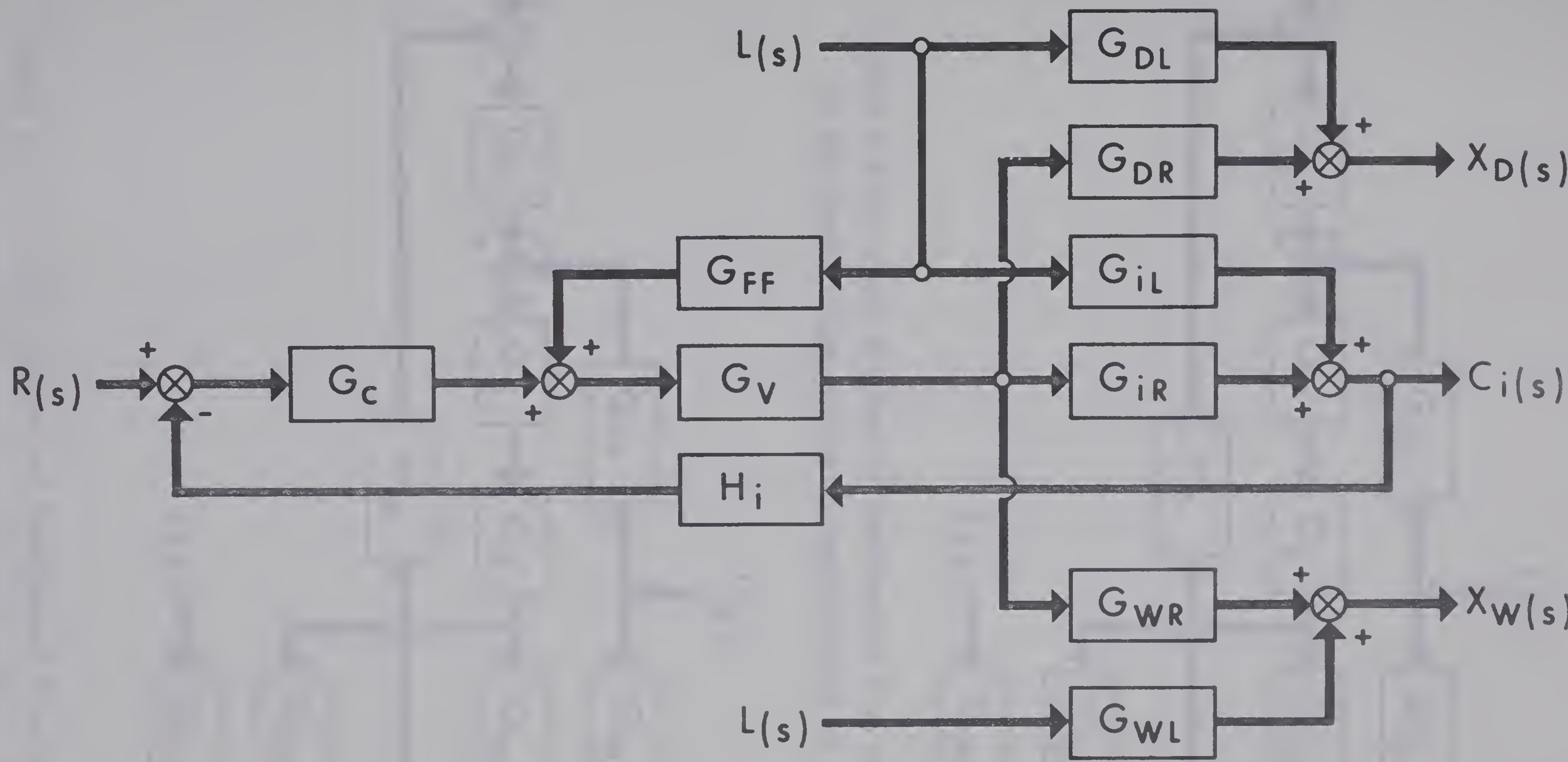


Figure 6.3-9 Block Diagram of Feedforward Plus Feedback Control of the Liquid Temperature (or Composition) on an Intermediate Tray by Manipulation of Reflux Flow

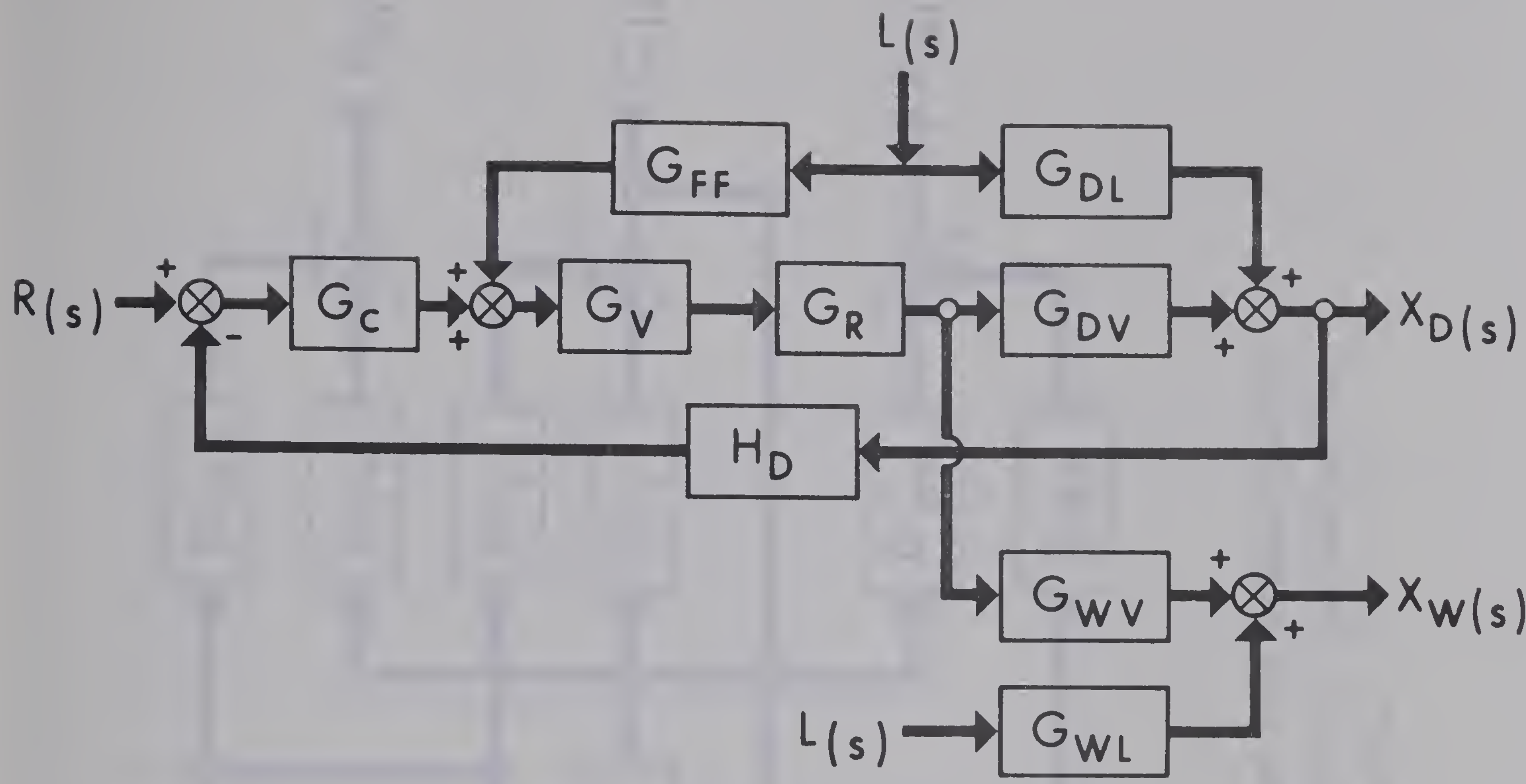


Figure 6.3-10 Block Diagram of Feedforward Plus Feedback Control of Top Product Composition by Manipulation of Steam Flow

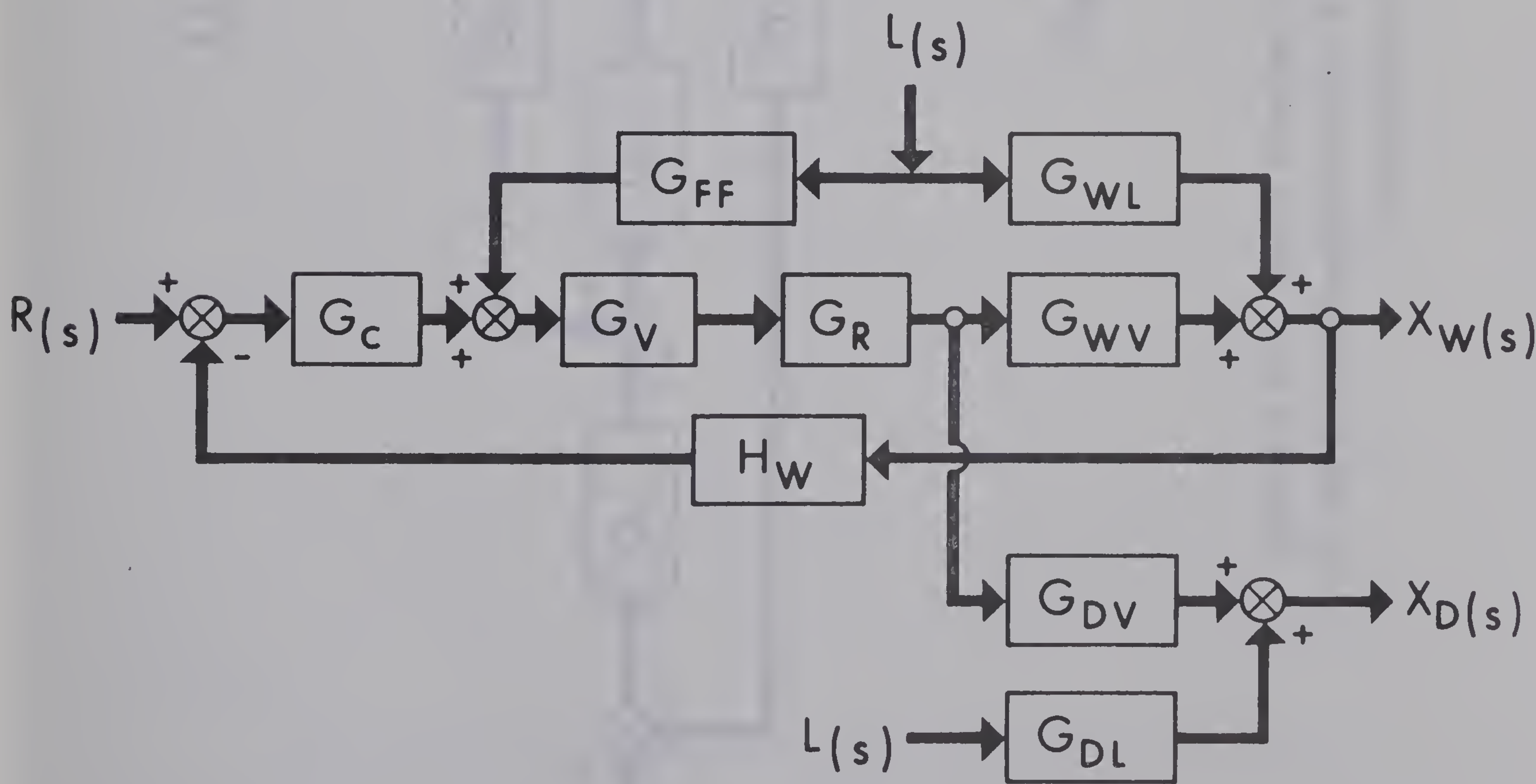
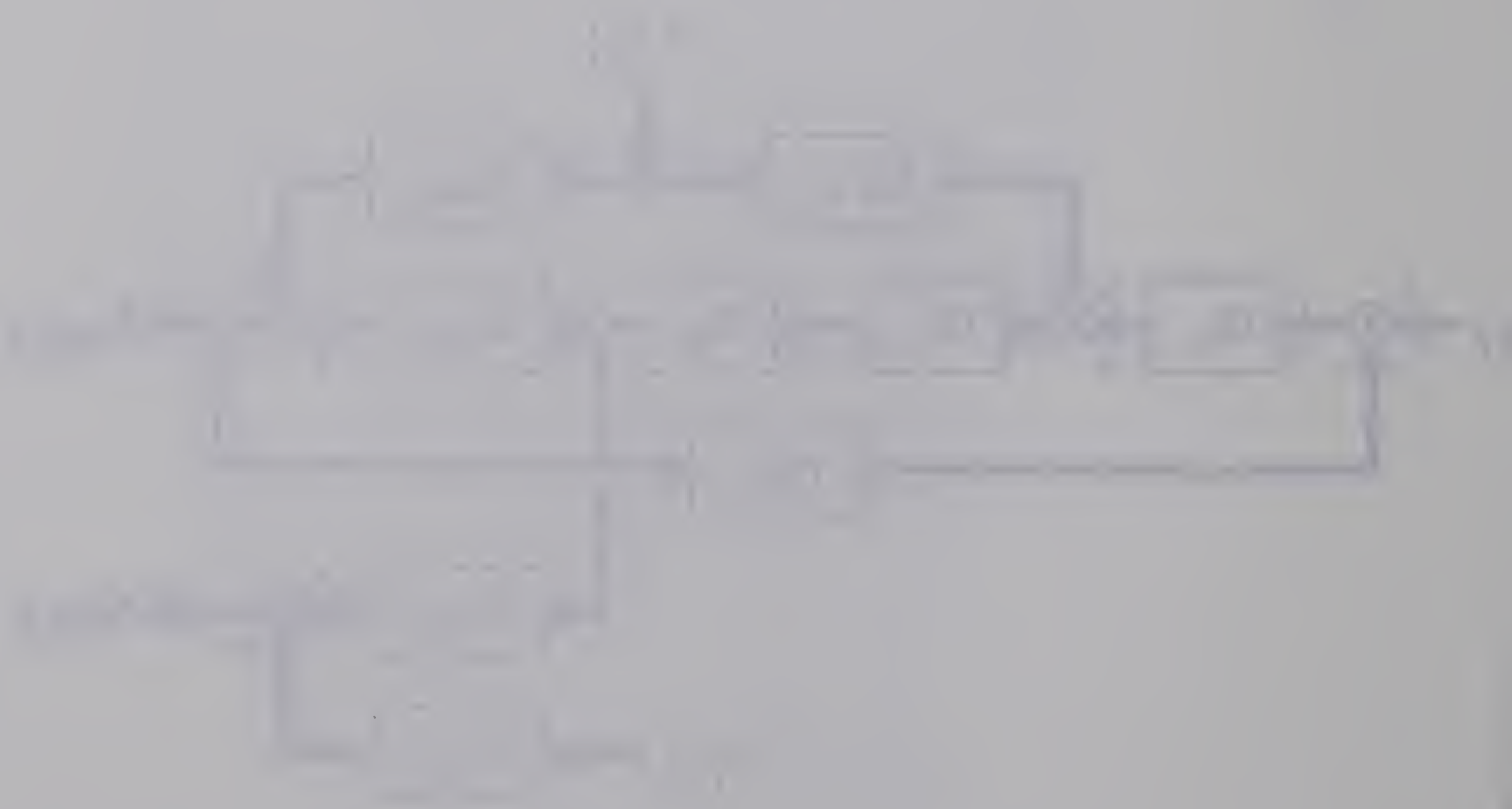


Figure 6.3-11 Block Diagram of Feedforward Plus Feedback Control of Bottom Product Composition by Manipulation of Steam Flow



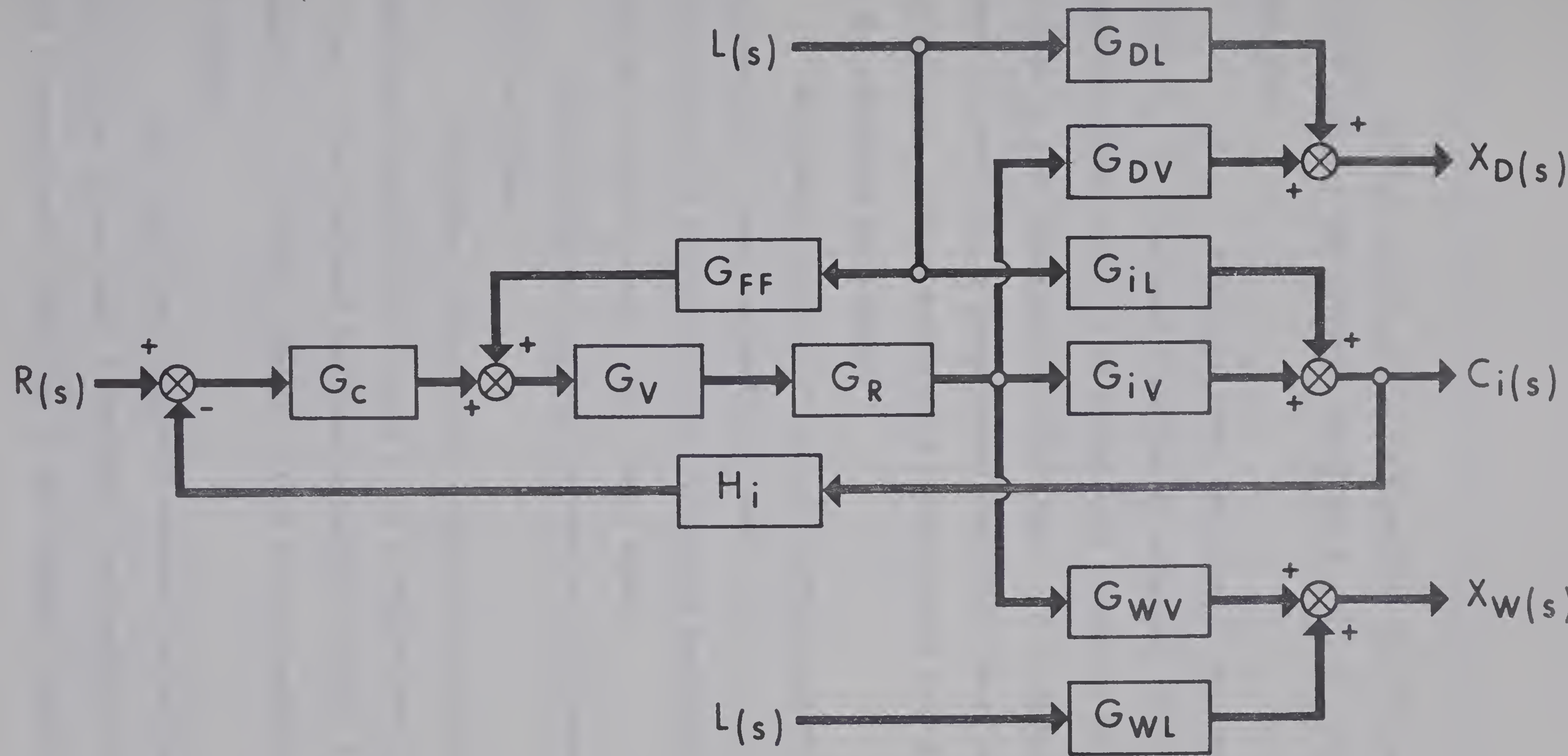


Figure 6.3-12 Block Diagram of Feedforward Plus Feedback Control of the Liquid Temperature (or Composition) on an Intermediate Tray by Manipulation of Steam Flow

K_V, K_R, K_{iL}, K_{iR}, K_{iV} in equations (6.3-1) through (6.3-6) are the gains of the transfer functions G_V, G_R, G_{iL}, G_{iR} and G_{iV} respectively.

For all simulation runs, the gain of the feedforward controller K_{FF} is calculated according to equations (6.3-1) through (6.3-6), depending on the case, so no offset will result in the controlled variable of the feedforward control loop. If a feedback control loop is added, in principle, a proportional controller would suffice. In a real process, perfect feedforward control would not be possible due to the following two reasons:

- The dynamic behavior of the real process may not be perfectly described by a linear mathematical model. This is due to the nonlinear nature of the distillation column and uncertainty in the determination of coefficients of the linear model.

- The existence of possible undetected disturbances in the distillation column.

Therefore, offset in the controlled variable will exist if feedforward control only is used or if a proportional controller alone is used in the combined feedforward-feedback control scheme. The necessity of utilizing integral action in the feedback control loop is obvious.

The simulation study will examine the performance of the distillation column under feedforward plus feedback control using not only a proportional controller in the feedback loop but also a proportional

plus integral controller in addition to feedforward compensation.

6.4 Results

As a complete set of transfer functions for the process is available, the transient response can be evaluated for various controller settings and the best controller constants are determined by trial and error. Unless otherwise noted, all runs were performed using a proportional plus integral (PI) feedback controller which can be represented as:

$$G_c = K_c\left(1 + \frac{1}{\tau_I s}\right)$$

Derivative action was not investigated as the temperature measurement usually is a noisy signal and the noise is amplified by derivative action. Furthermore, work by Rose, Williams and co-workers (60,79) has shown that derivative action is ineffective in controlling a distillation column. Their simulation results showed that the only action of derivative control was to add noise to the corrections called for by the proportional plus integral control.

All simulations in this control study have been done using the digital simulation language S/360 CSMP. Listings of some typical programs appear in Appendix C. Detailed discussions of these programs are not given here as the preparation of these CSMP statements is a rather straightforward procedure. However, some pertinent features of the S/360 CSMP which have been used to advantage to reduce the

computing time will be mentioned here:

- As a guide, the total time of each simulation run (FINTIM) has been limited to 120.0 minutes. For all practical purposes, the complete transient response dies out after this amount of time has been elapsed. A longer total time would only serve to lengthen the computing time. Therefore, in evaluating the results, the integral of the squared error was computed from 0 to 120.0 minutes.

- To reduce unnecessary calculations when instability occurs in the transient response, the simulation run will be terminated even before the total time of the run is elapsed, if the I.S.E. is larger than a predetermined value. This value, which varies from tray to tray is selected by experience.

- Selection of the integration method and the integration interval has been given careful consideration to further reduce the computing time required. During early runs of the simulation study where it is not necessary to obtain particularly accurate transient responses, the fixed-step Runge-Kutta routine (RKSFX) has been used. The integration interval has been set at 0.10 minutes as it will provide relatively fast execution while maintaining enough accuracy. With controller settings near or at the optimum values, high accuracy is required, so the variable-step Runge-Kutta routine (RKS) is used. This procedure has the advantage of ensuring a satisfactory solution with the maximum possible step size, but sometimes at the cost of excessive computing time. Whenever the RKS routine is used, the integration

interval is set arbitrarily at 0.20 minutes.

Although the I.S.E. has been chosen as the overall performance criterion to facilitate the determination of optimum controller settings, other dynamic performance criteria such as maximum deviation, offset and settling time will also be considered in any final judgement of the control system performance. Unlike maximum deviation and offset where standard definitions can be found in common control textbooks (23,29), the definition of the settling time is somewhat arbitrary and therefore, it requires some explanation. During this investigation, the settling time is defined as:

(i) If there is no offset in the transient response, the settling time is the time required for the amplitude of oscillation to remain within $\pm$ 5 per cent of the maximum deviation.

(ii) If there is offset in the system, the settling time is the time required for the system response to remain within $\pm$ 5 per cent of the final value.

6.4.1 Simulation Results Using Data from the University of Delaware Distillation Column

To study the control performance of the column, all the transfer functions in the block diagrams given in Figures 6.3-1 through 6.3-12 must be known. The dynamic relations of the distillation process itself were listed in Tables 5.3-1, 5.3-2 and 5.3-3. The transfer functions representing the dynamics of the reboiler, the composition measuring element and the control valve have to be evaluated.

Data reported by Gerster et al (40) revealed that there exists a lag of 30 seconds between the time at which the set point of the steam controller is changed and the time when the vapor flow reaches the column, so a first order transfer function with a time constant equal to 0.5 minutes was employed to describe the dynamics of the reboiler,

$$G_R = \frac{V(s)}{S(s)} = \frac{K_R}{0.5s + 1}$$

where V(s) and S(s) are the Laplace transforms of the reboil vapor rate and the steam flow rate respectively. During all simulations, on the basis of calculations from Gerster's data, the constant K_R relating the steam condensation rate and the boil up rate was taken as being equal to

$$K_R = 5.0 \ \frac{\text{lb. mole/min. of reboil vapor rate}}{\text{lb./min. of steam rate}}$$

Gerster et al also reported that a delay of 1.0 minutes is required for the liquid sample to flow from the sampling point to a common point where a simultaneous collection of all samples was made. Thus, it can be assumed that the error E(s) transmitted to the controller is related to e(s), the true error, by the following transfer function:

$$H_D = H_W = H_i = \frac{1}{1.0s + 1}$$

The transfer function of the control valve was taken as unity, that is, $G_V = 1.0$. This assumption of only a gain transfer function is very reasonable as in general, the dynamics of the control valve are very fast compared to the dynamics of the process itself.

Only single point sampling of top product composition, bottom product composition and composition of the liquid on an intermediate tray were actually studied in this work. During this investigation, to simplify the computations, it was assumed that these compositions can be measured and fed back to the controller continuously.

A stepwise variation in feed composition of 5 mole per cent acetone was used as the forcing function for the series of simulations carried out for a wide range of controller settings. The results which give the minimum I.S.E. value in the composition of the controlled variable are presented in graphical and tabular forms. Typical results are exemplified by Figures 6.4-1 to 6.4-25 which illustrate the control behavior of the column for composition control of trays 7 and 9 by manipulation of reflux flow and trays 1, 3, 7 by manipulation of reboil vapor rate. The remaining results from the simulations are tabulated. This is considered to be the most compact and direct method of illustrating the effects of the control point on the distillation column performance. The results are tabulated in Tables 6.4-1 through 6.4-14. In all the graphs and tables presented in this section, the following units apply:

X_D	:	mole per cent acetone
X_W	:	mole per cent acetone
X_i	:	mole per cent acetone
Maximum deviation (M.D.)	:	mole per cent acetone
Offset (Off.)	:	mole per cent acetone
Settling time (S.T.)	:	minutes
Integral time (τ_I)	:	minutes
K_c	:	$\frac{\text{lb.mole/min.}}{\text{mole per cent}}$
K_{FF}	:	$\frac{\text{lb.mole/min.}}{\text{mole per cent}}$

X_D, X_W and X_i are the deviation variables.

It should be noted that composition control by manipulation of reboil vapor rate necessitates the use of a negative feedback controller gain.

The following cases were examined in this part of the investigation:

A. Manipulation of reflux flow

(i) Feedback control of the liquid composition on an intermediate tray.

Summary of results - Table 6.4-1

Typical column responses - Figures 6.4-1 and 6.4-2

(ii) Feedforward plus feedback control of the liquid composition on an intermediate tray using a proportional controller in the feed-

back loop.

Summary of results - Table 6.4-2

Typical column responses - Figures 6.4-3 and 6.4-4

(iii) Feedforward plus feedback control of the liquid composition on an intermediate tray using a PI controller in the feedback loop, τ_I = 100.0 minutes.

Summary of results - Table 6.4-3

Typical column responses - Figures 6.4-5 and 6.4-6

(iv) Feedforward plus feedback control of the liquid composition on an intermediate tray using a PI controller in the feedback loop, τ_I = 10.0 minutes.

Summary of results - Table 6.4-4

Typical column responses - Figures 6.4-7 and 6.4-8

(v) Feedforward plus feedback control of the liquid composition on an intermediate tray using a PI controller in the feedback loop, τ_I = 1.0 minutes.

Summary of results - Table 6.4-5

Typical column responses - Figures 6.4-9 and 6.4-10

(vi) Feedback control and combined feedforward-feedback control of top product composition.

Summary of results - Table 6.4-6

(vii) Feedback control and combined feedforward-feedback control of bottom product composition.

Summary of results - Table 6.4-7

B. Manipulation of steam flow

(i) Feedback control of the liquid composition on an intermediate tray

Summary of results	- Table 6.4-8
Typical column responses	- Figures 6.4-11, 6.4-12 and 6.4-13

(ii) Feedforward plus feedback control of the liquid composition on an intermediate tray using a proportional controller in the feedback loop.

Summary of results	- Table 6.4-9
Typical column responses	- Figures 6.4-14, 6.4-15 and 6.4-16

(iii) Feedforward plus feedback control of the liquid composition on an intermediate tray using a PI controller in the feedback loop, τ_I = 100.0 minutes.

Summary of results	- Table 6.4-10
Typical column responses	- Figures 6.4-17, 6.4-18 and 6.4-19

(iv) Feedforward plus feedback control of the liquid composition on an intermediate tray using a PI controller in the feedback loop, τ_I = 10.0 minutes.

Summary of results	- Table 6.4-11
Typical column responses	- Figures 6.4-20, 6.4-21 and 6.4-22

(v) Feedforward plus feedback control of the liquid composition on an intermediate tray using a PI controller in the feedback loop τ_I = 1.0 minutes.

Summary of results - Table 6.4-12

Typical column responses - Figures 6.4-23, 6.4-24 and 6.4-25

(vi) Feedback control and combined feedforward-feedback control of top product composition.

Summary of results - Table 6.4-13

(vii) Feedback control and combined feedforward-feedback control of bottom product composition.

Summary of results - Table 6.4-14

6.4.2 Simulation Results Using Data from the University of Alberta Distillation Column

The transfer functions representing the dynamics of the University of Alberta distillation column for changes in feed flow, reflux flow and steam flow were tabulated in Tables 5.4-2, 5.4-3, and 5.4-4. It should be mentioned here that Table 5.4-4 actually listed the transfer function relating the liquid temperature on intermediate trays, top and bottom product compositions for changes in steam flow rate, that is the dynamics of the reboiler has been included in these transfer functions, therefore, the reboiler transfer function has been taken as equal to 1.0, G_R = 1.0.

Table 6.4-1

Feedback Control of the Liquid Composition on an Intermediate Tray

by Manipulation of Reflux Flow

(University of Delaware Column)

Control tray		1	3	7	9
Optimum controller settings	K_c	0.11	0.13	10.0	10.0
	τ_I	9.0	9.0	1.5	1.8
X_D	M.D.	-2.01	-1.94	-0.84	-0.72
	Off.	-0.50	-0.30	0.62	0.18
	S.T.	52.	49.	44.	49.
	I.S.E.	76.05	56.06	39.92	8.051
X_W	M.D.	6.84	7.11	8.05	7.57
	Off.	6.84	7.11	8.05	7.57
	S.T.	28.	27.	24.	19.
	I.S.E.	4988.	5279.	6953.	6270.
X_i	M.D.	3.14	3.67	0.18	0.13
	Off.	0.00	0.00	0.00	0.00
	S.T.	50.	34.	2.	2.
	I.S.E.	27.69	21.55	0.0005	0.0003

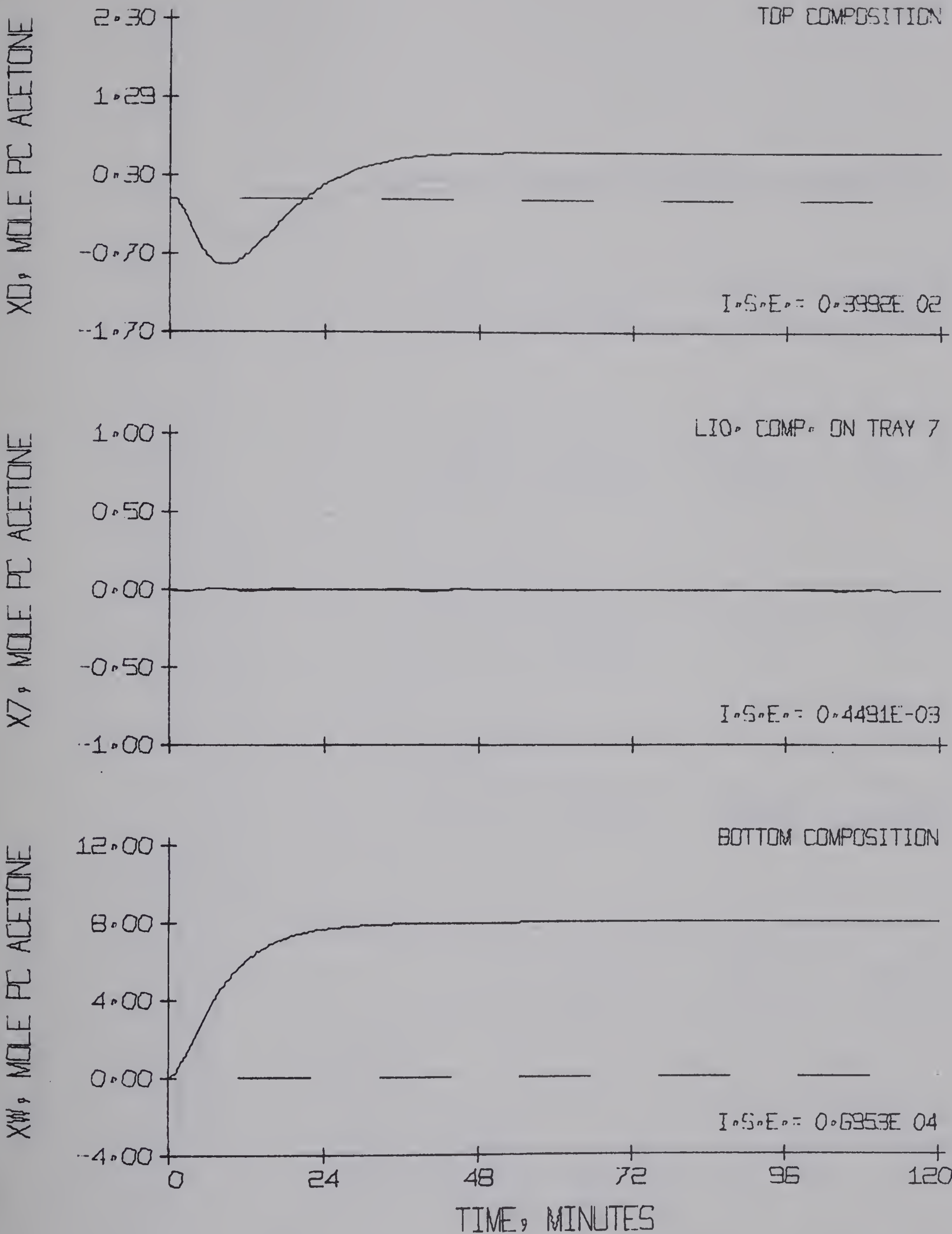


Figure 6.4-1 Feedback Control of the Liquid Composition on Tray 7
by Manipulation of Reflux Flow
(University of Delaware Column)

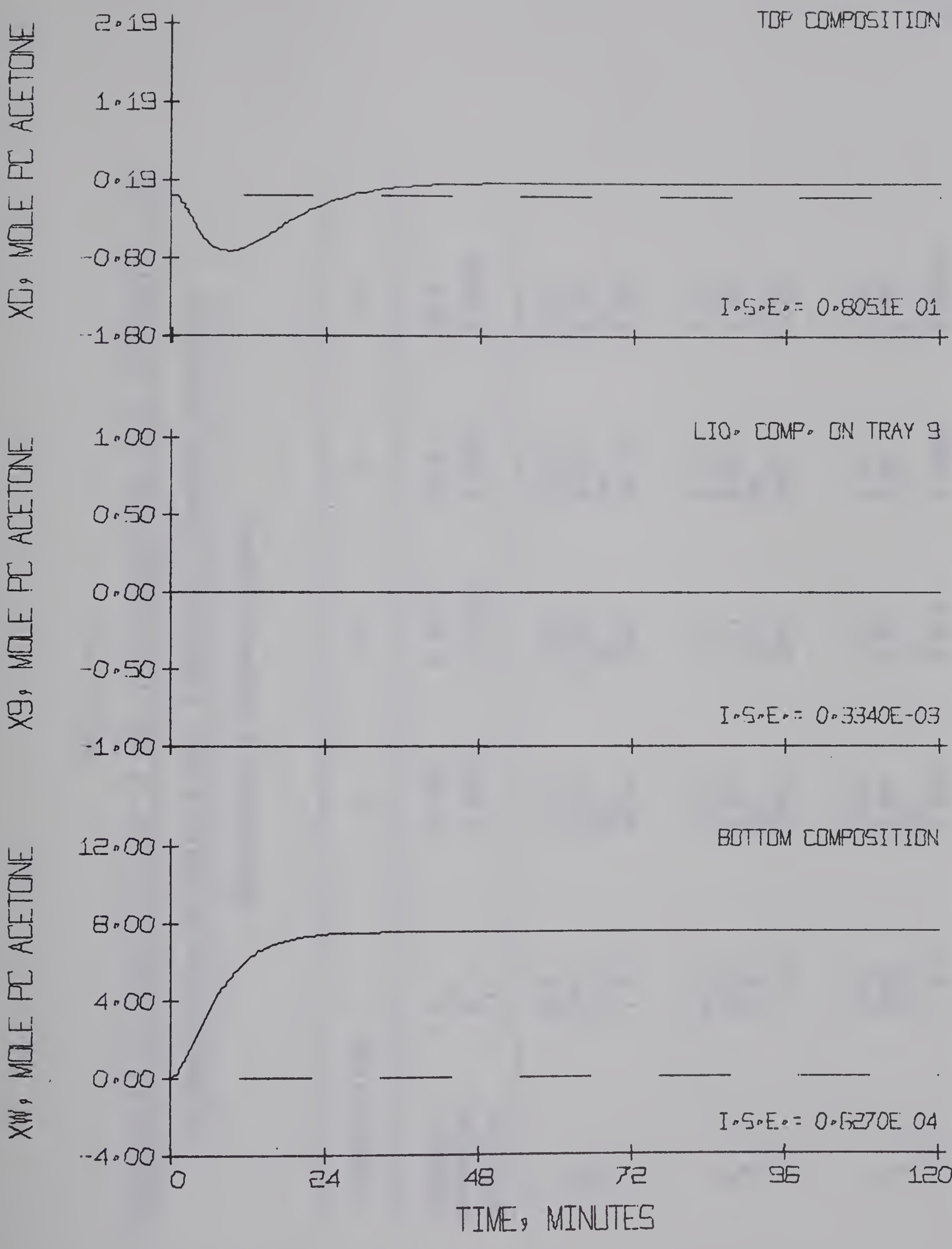


Figure 6.4-2 Feedback Control of the Liquid Composition on Tray 9 by Manipulation of Reflux Flow (University of Delaware Column)

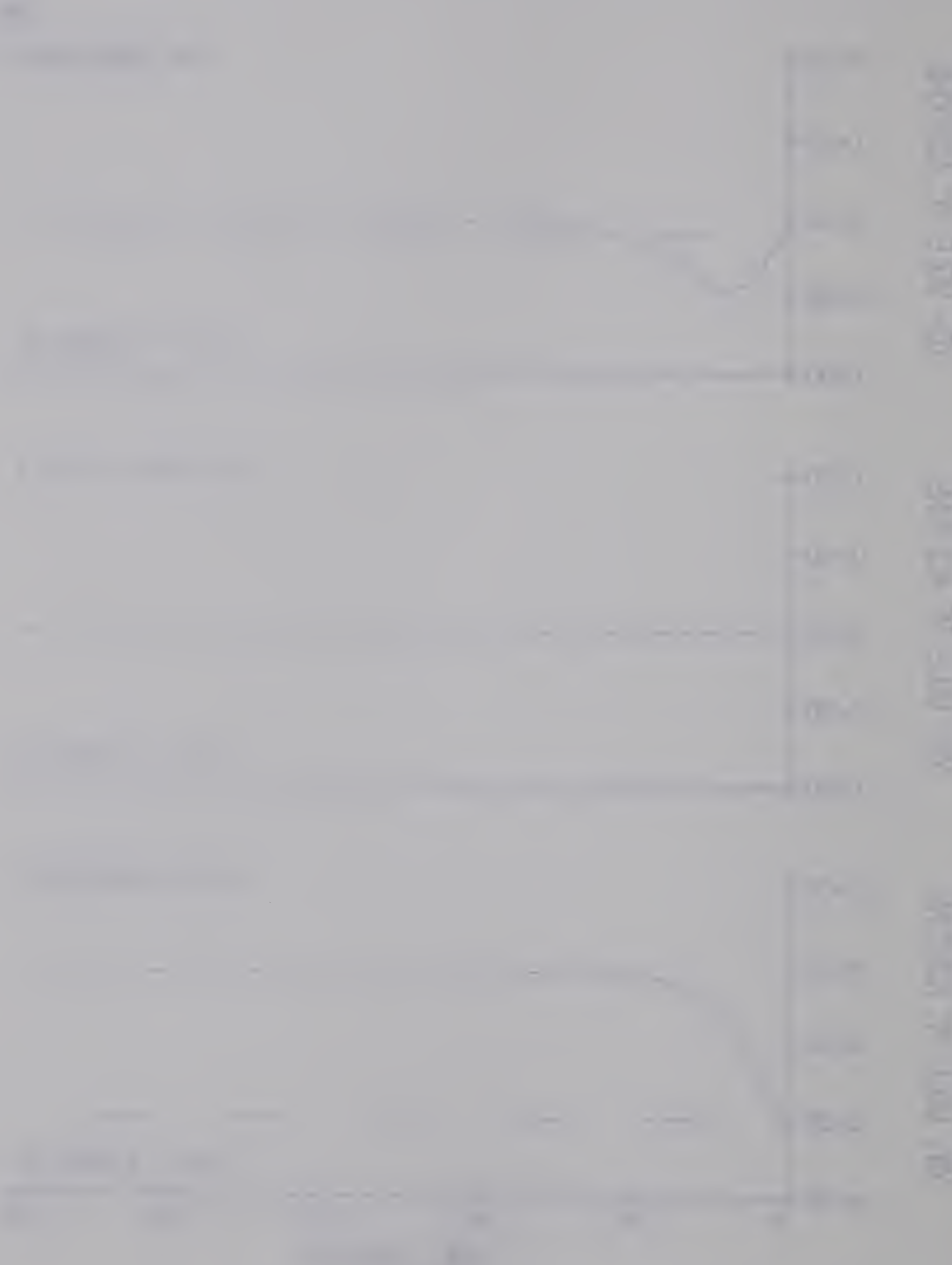


Table 6.4-2

Feedforward Plus Feedback Control of the Liquid Composition on an Intermediate Tray

by Manipulation of Reflux Flow - Proportional Feedback Controller

(University of Delaware Column)

Control Tray		1	3	7	9
Optimum controller settings	K_c	0.108	0.126	10.0	10.0
	K_{FF}	-0.0352	-0.0339	-0.0276	-0.0306
X_D	M.D.	-1.91	-1.99	-0.85	-0.72
	Off.	-0.50	-0.30	0.62	0.18
	S.T.	50.	49.	44.	48.
	I.S.E.	8294.	6184.	39.91	8.052
X_W	M.D.	6.84	7.12	8.05	7.57
	Off.	6.84	7.11	8.05	7.57
	S.T.	28.	27.	24.	19.
	I.S.E.	4958.	5246.	6953.	6270.
X_i	M.D.	1.06	1.78	0.03	-0.01
	Off.	0.00	0.00	0.00	0.00
	S.T.	25.	15.	0.	0.
	I.S.E.	2.290	3.254	0.0000	0.0000

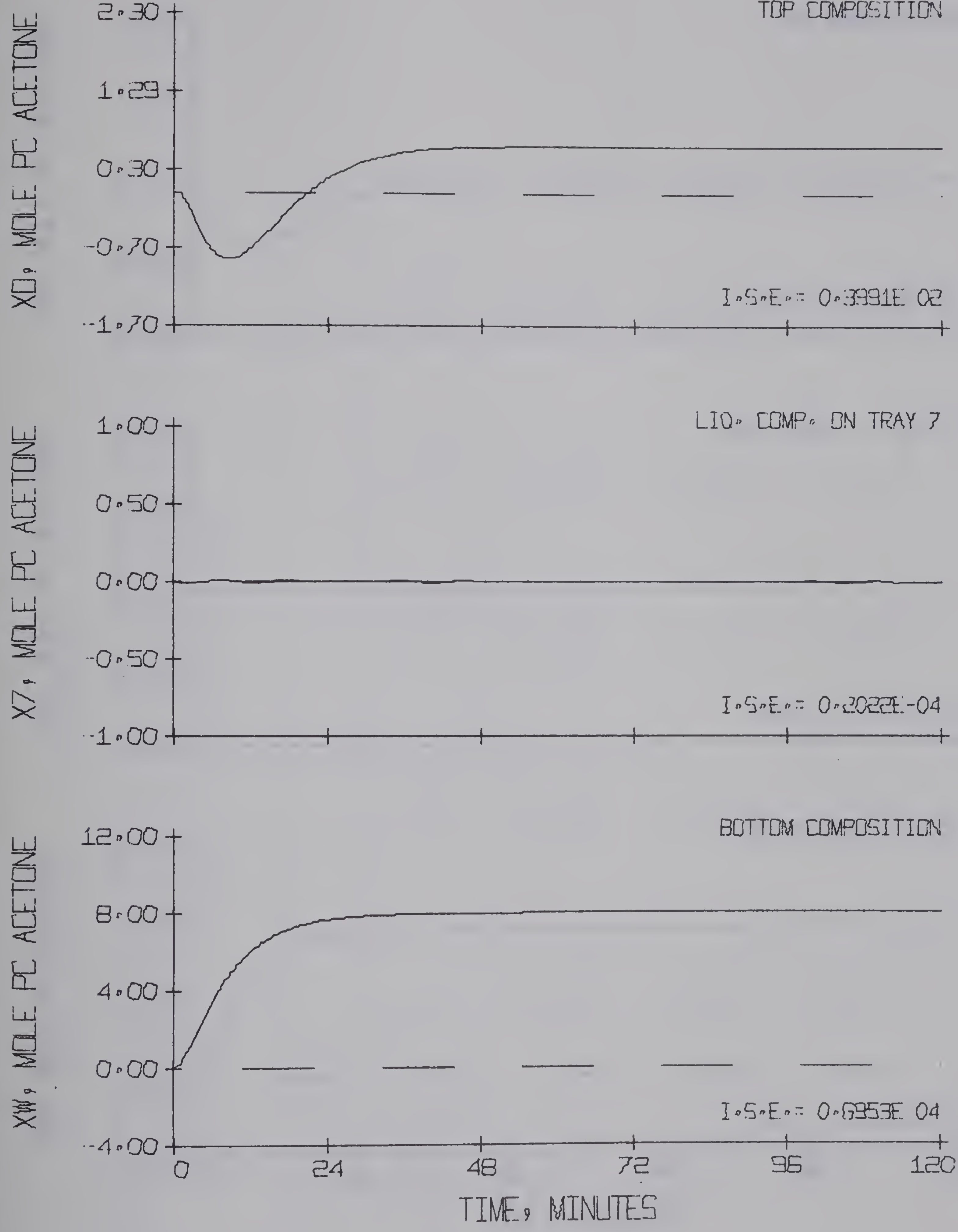


Figure 6.4-3 Feedforward Plus Feedback Control of the Liquid Composition on Tray 7 by Manipulation of Reflux Flow - Proportional Feedback Controller (University of Delaware Column)

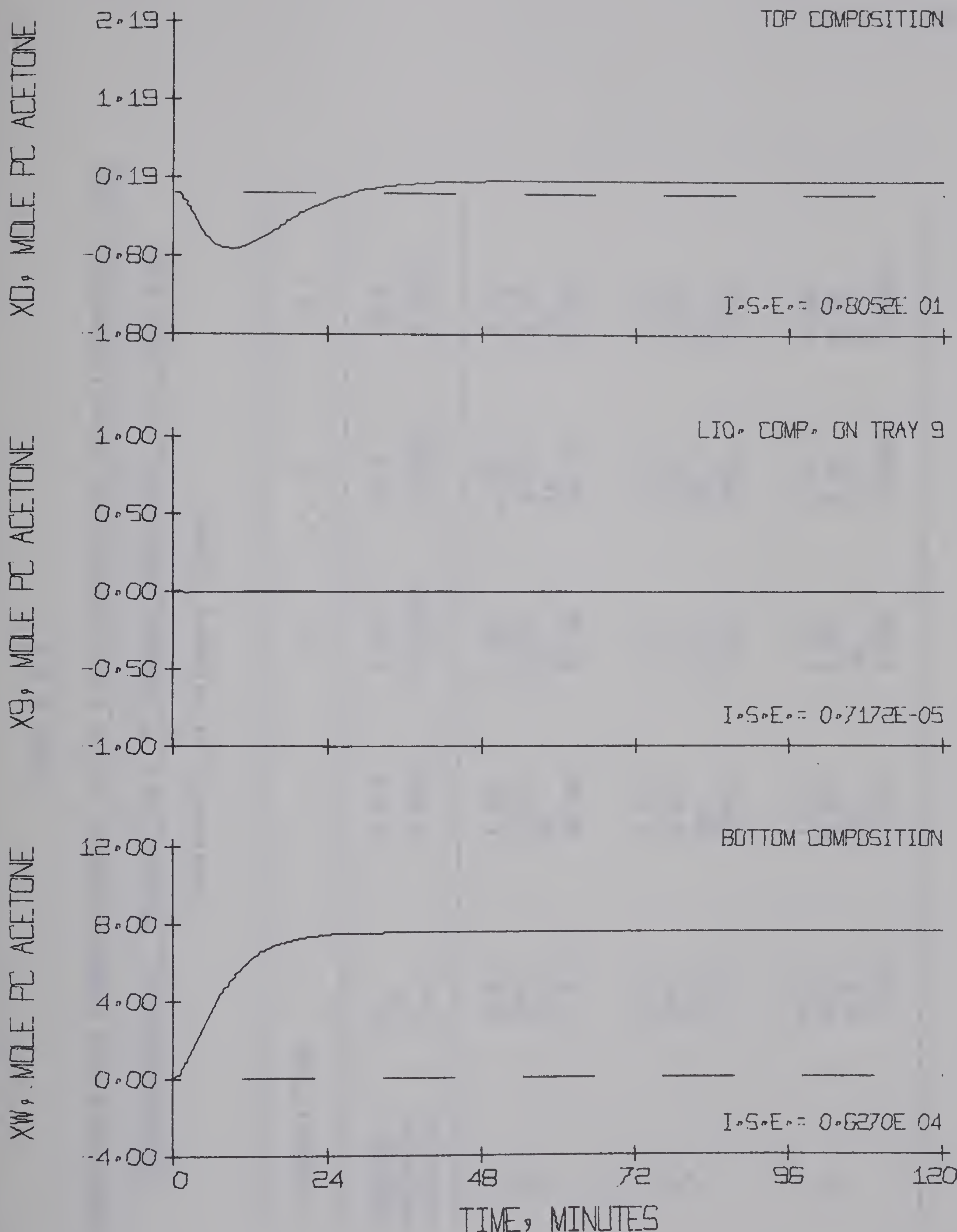


Figure 6.4-4 Feedforward Plus Feedback Control of the Liquid Composition on Tray 9 by Manipulation of Reflux Flow - Proportional Feedback Controller (University of Delaware Column)

Table 6.4-3

Feedforward Plus Feedback Control of the Liquid Composition on an Intermediate Tray by Manipulation of Reflux Flow - PI Feedback Controller, τ_I = 100.0 min.

(University of Delaware Column)

Control Tray		1	3	7	9
Optimum controller settings	K_c	0.115	0.121	10.0	10.0
	K_{FF}	-0.0352	-0.0339	-0.0276	-0.0306
X_D	M.D.	-1.92	-1.99	-0.85	-0.72
	Off.	-0.50	-0.30	0.62	0.18
	S.T.	52.	50.	44.	49.
	I.S.E.	84.62	62.66	39.91	8.051
X_W	M.D.	6.84	7.11	8.05	7.62
	Off.	6.84	7.11	8.05	7.57
	S.T.	29.	27.	24.	19.
	I.S.E.	4945.	5237.	6953.	6270.
X_i	M.D.	1.07	1.78	0.00	0.00
	Off.	0.00	0.00	0.00	0.00
	S.T.	26.	16.	0.	0.
	I.S.E.	2.317	3.299	0.0000	0.0000

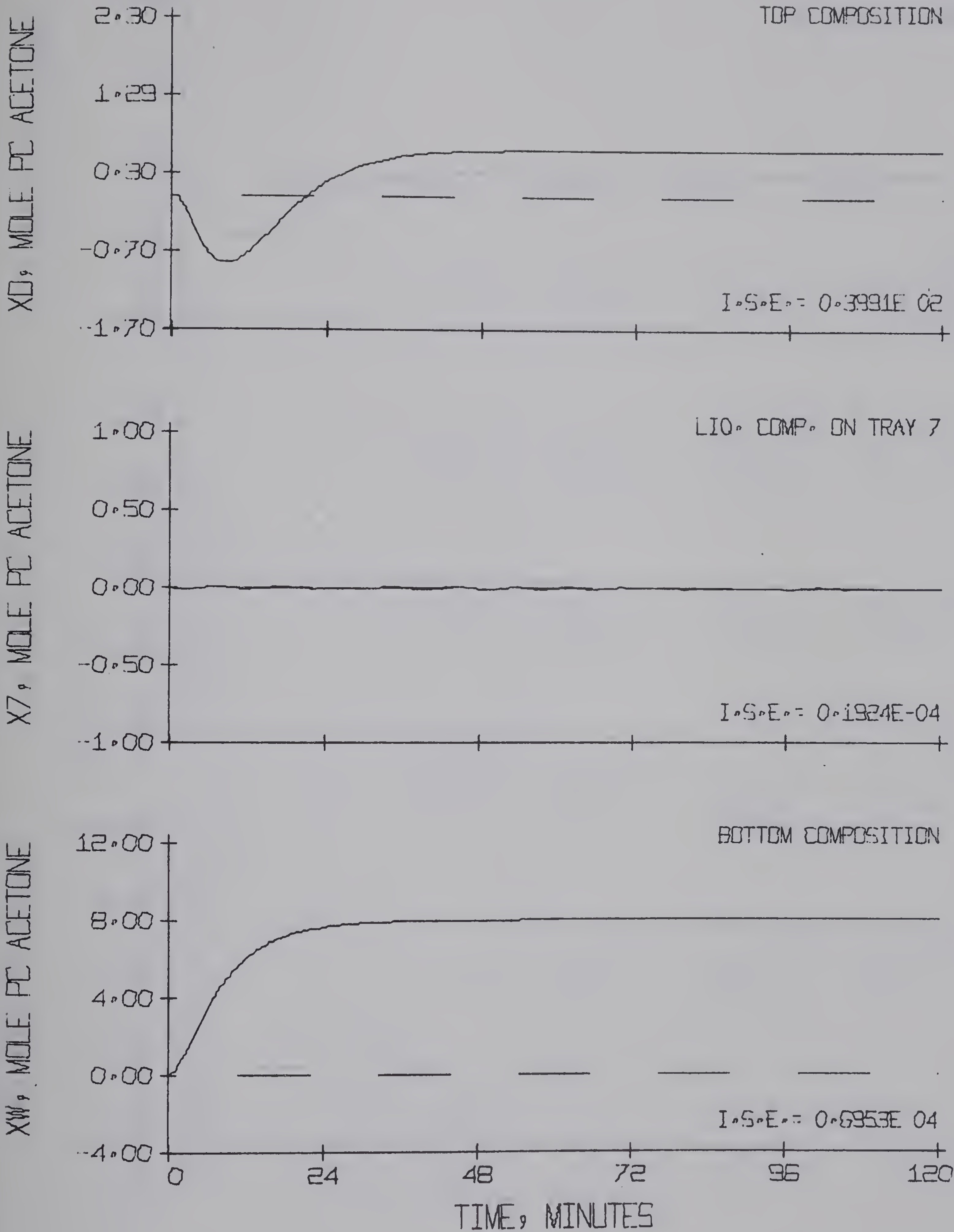


Figure 6.4-5 Feedforward Plus Feedback Control of the Liquid Composition on Tray 7 by Manipulation of Reflux Flow - PI Feedback Controller, τ_I = 100.0 min. (University of Delaware Column)

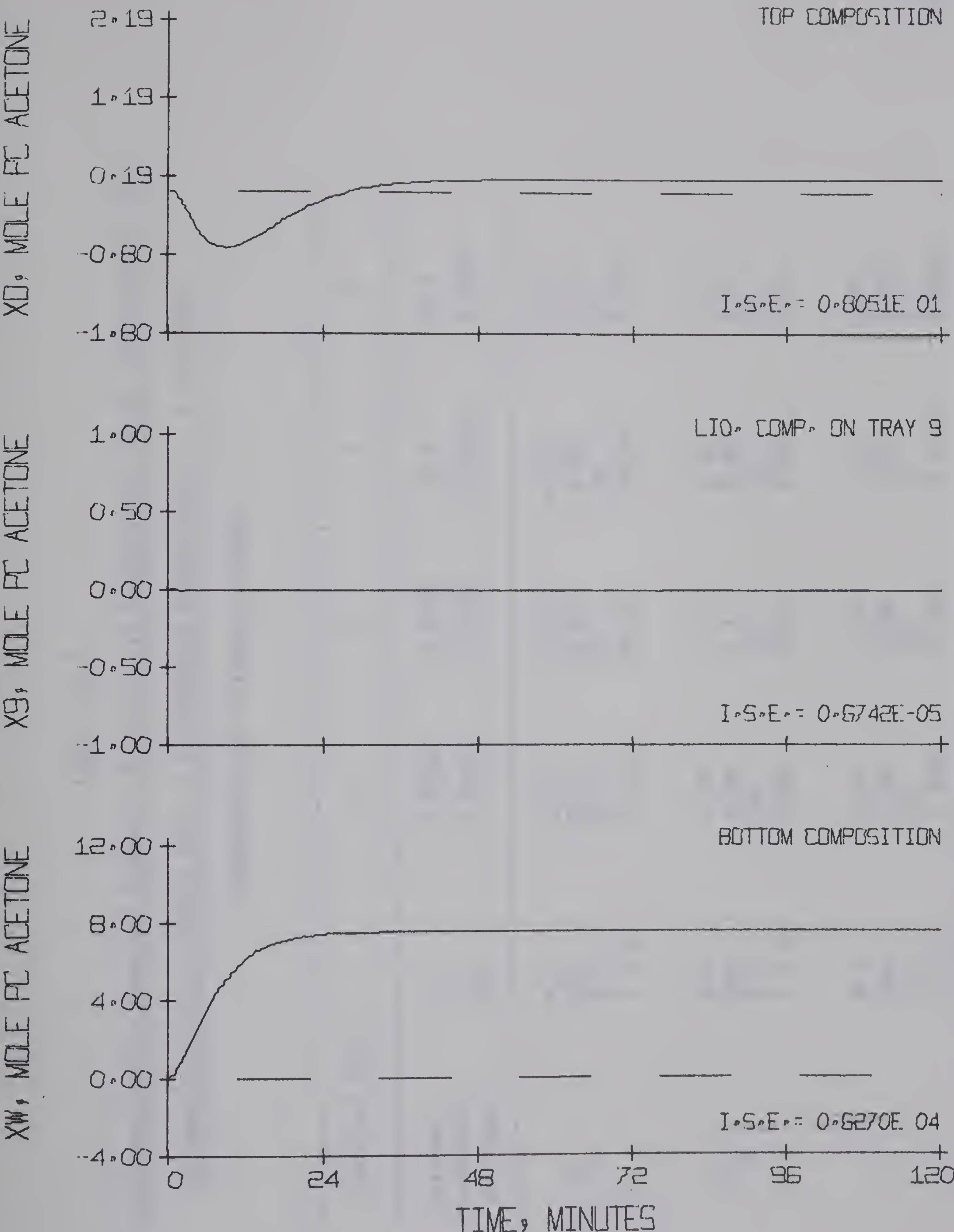


Figure 6.4-6 Feedforward Plus Feedback Control of the Liquid Composition on Tray 9 by Manipulation of Reflux Flow - PI Feedback Controller, τ_I = 100.0 min. (University of Delaware Column)

Table 6.4-4

Feedforward Plus Feedback Control of the Liquid Composition on an Intermediate Tray by Manipulation of Reflux Flow - PI Feedback Controller, τ_I = 10.0 min.

(University of Delaware Column)

Control Tray		1	3	7	9
Optimum controller settings	K_c	0.0094	0.0108	10.0	10.0
	K_{FF}	-0.0352	-0.0339	-0.0276	-0.0306
X_D	M.D.	-2.05	-2.02	-0.85	-0.72
	Off.	-0.50	-0.30	0.62	0.18
	S.T.	51.	51.	44.	49.
	I.S.E.	87.54	64.76	39.92	8.050
X_W	M.D.	6.84	7.11	8.05	7.57
	Off.	6.84	7.11	8.05	7.57
	S.T.	29.	27.	23.	19.
	I.S.E.	4940.	5233.	6953.	6270.
X_i	M.D.	1.06	1.80	0.03	-0.01
	Off.	0.00	0.00	0.00	0.00
	S.T.	34.	22.	0.	0.
	I.S.E.	2.648	3.762	0.0000	0.0000

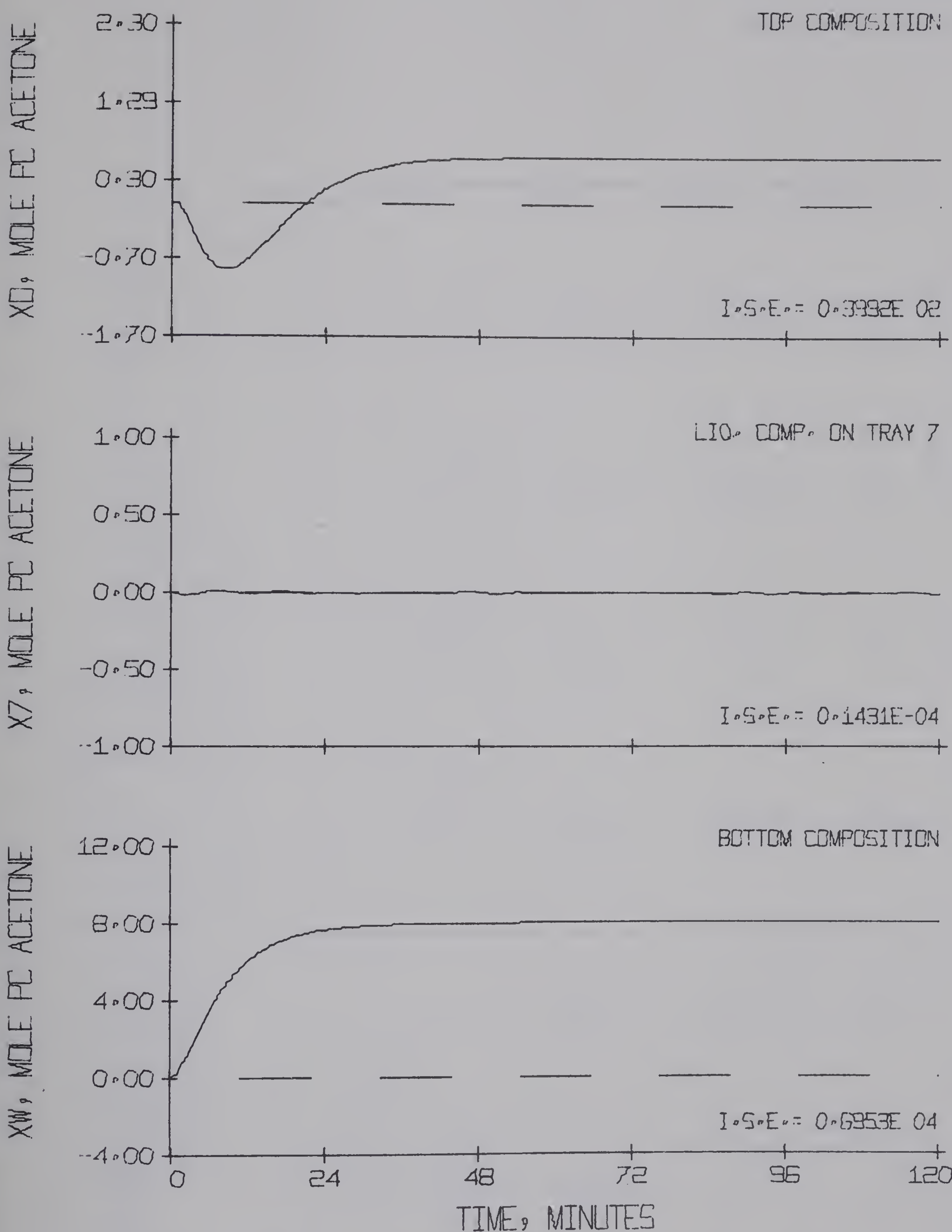


Figure 6.4-7 Feedforward Plus Feedback Control of the Liquid Composition on Tray 7 by Manipulation of Reflux Flow - PI Feedback Controller, τ_I = 10.0 min. (University of Delaware Column)

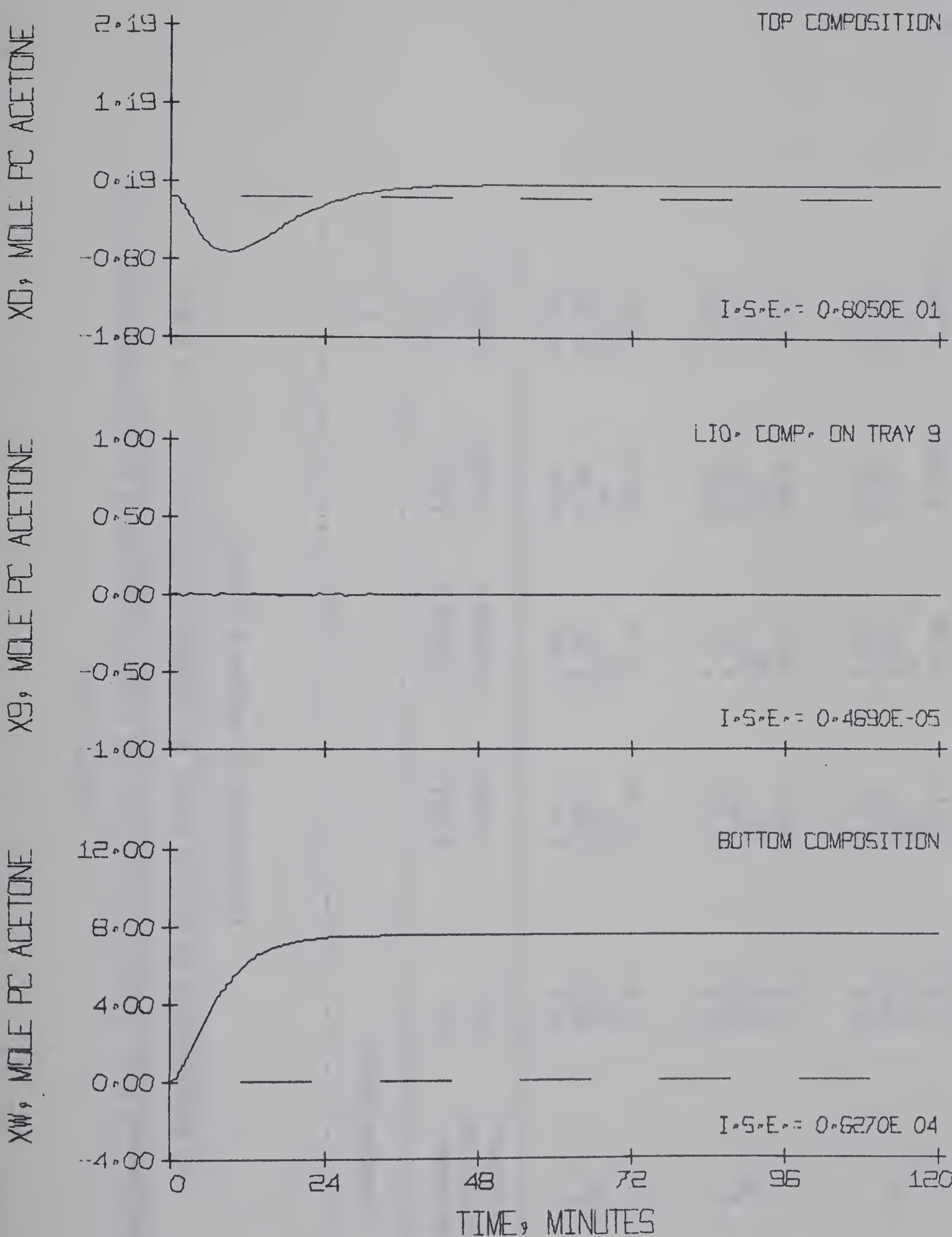


Figure 6.4-8 Feedforward Plus Feedback Control of the Liquid Composition on Tray 9 by Manipulation of Reflux Flow - PI Feedback Controller, τ_I = 10.0 min. (University of Delaware Column)

Table 6.4-5

Feedforward Plus Feedback Control of the Liquid Composition on an Intermediate Tray by Manipulation of Reflux Flow - PI Feedback Controller, τ_I = 1.0 min.

(University of Delaware column)

Control Tray		1	3	7	9
Optimum controller settings	K_c	0.0041	0.0074	10.0	10.0
	K_{FF}	-0.0352	-0.0339	-0.0276	-0.0306
X_D	M.D.	-2.01	-2.40	-0.85	-0.72
	Off.	-0.50	-0.30	0.62	0.18
	S.T.	61.	61.	44.	49.
	I.S.E.	93.36	72.59	39.92	8.05
X_W	M.D.	7.03	7.11	8.05	7.57
	Off.	6.84	7.11	8.05	7.57
	S.T.	41.	39.	24.	19.
	I.S.E.	4932.	5227.	6953.	6270.
X_i	M.D.	1.39	-2.47	-0.03	-0.01
	Off.	0.00	0.00	0.00	0.00
	S.T.	38.	37.	1.	1.
	I.S.E.	35.17	65.08	0.0000	0.0000

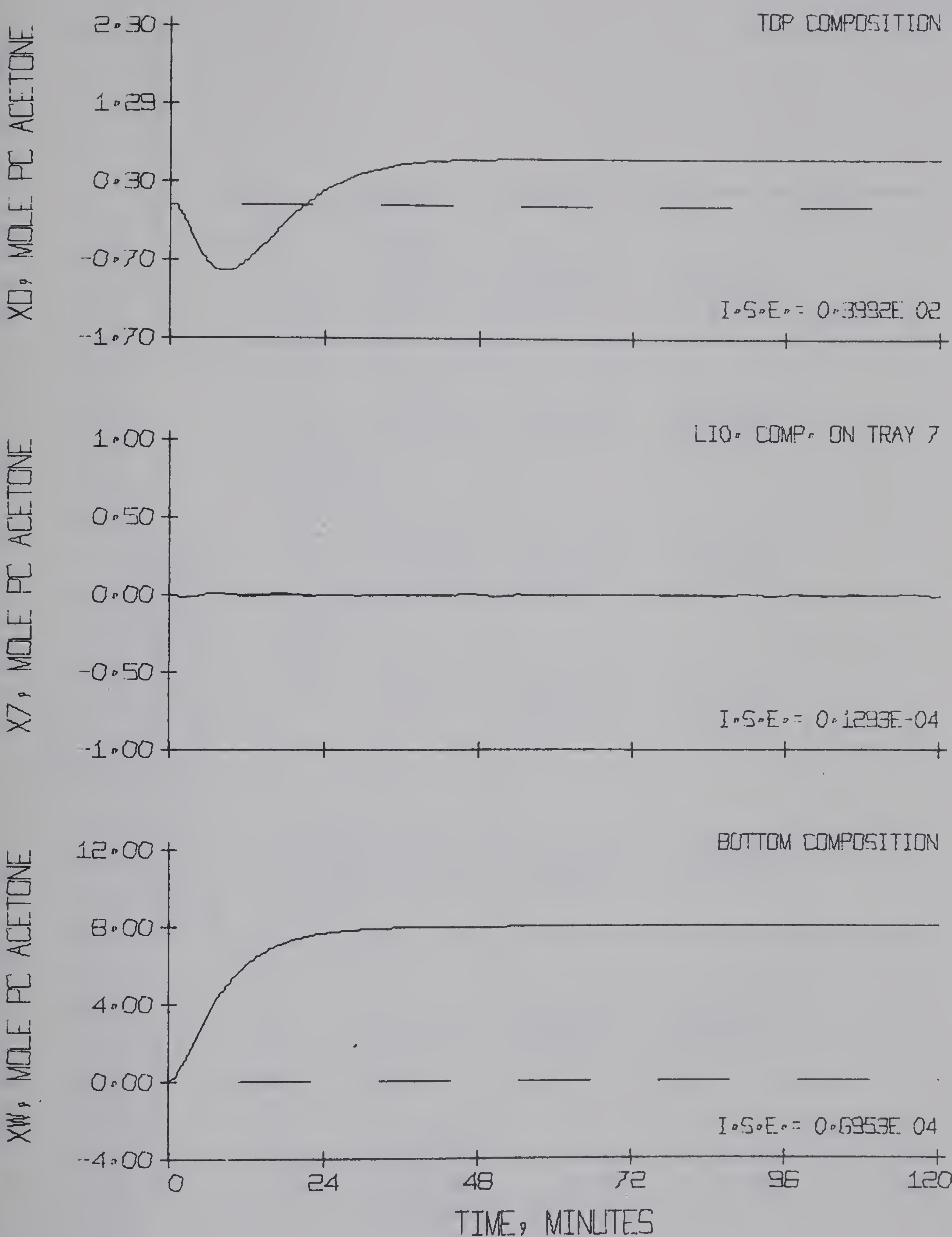


Figure 6.4-9 Feedforward Plus Feedback Control of the Liquid Composition on Tray 7 by Manipulation of Reflux Flow - PI Feedback Controller, τ_I = 1.0 min. (University of Delaware Column)

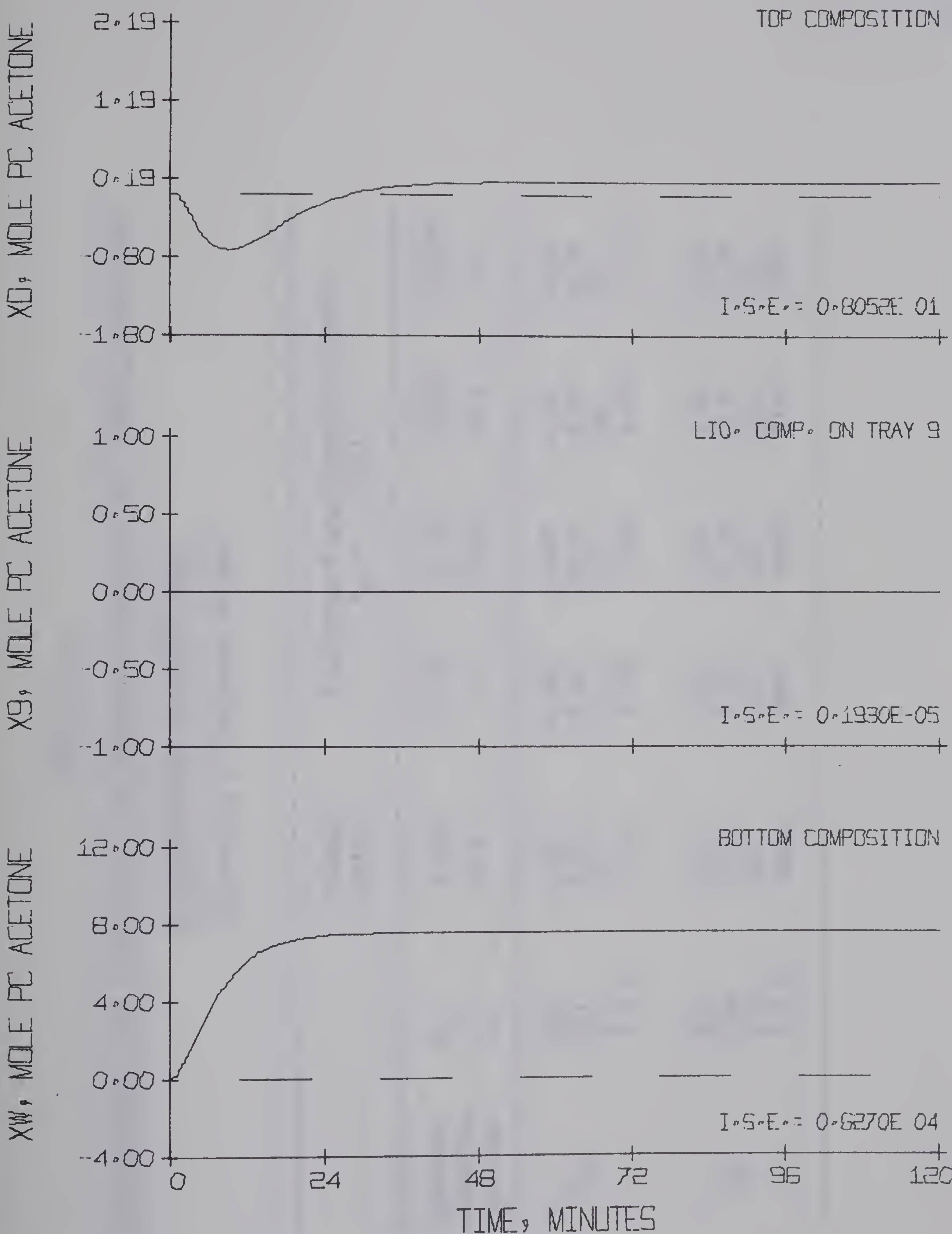


Figure 6.4-10 Feedforward Plus Feedback Control of the Liquid Composition on Tray 9 by Manipulation of Reflux Flow PI Feedback Controller, τ_I = 1.0 min. (University of Delaware Column)

Table 6.4-6

Feedback Control and Feedforward Plus Feedback Control of Top Product Composition

by Manipulation of Reflux Flow

(University of Delaware Column)

		Feedback Control	Feedforward plus Feedback Control $K_{FF} = -0.0318$			
Optimum controller settings	K_c	0.130	0.125	0.119	0.085	0.00006
	τ_I	12.0	∞	100.0	10.0	1.0
X_D	M.D.	-1.21	-0.66	-0.67	-0.70	-0.96
	Off.	0.00	0.00	0.00	0.00	0.00
	S.T.	43.	10.	10.	20.	32.
	I.S.E.	11.33	2.338	2.442	4.012	11.15
X_W	M.D.	8.21	7.65	7.67	7.97	7.41
	Off.	7.38	7.38	7.38	7.38	7.38
	S.T.	44.	14.	14.	24.	36.
	I.S.E.	6338.	6078.	6166.	6195.	5971.

Table 6.4.7

Feedback Control and Feedforward Plus Feedback Control of Bottom Product Composition

by Manipulation of Reflux Flow

(University of Delaware Column)

		Feedback Control	Feedforward plus Feedback Control $K_{FF} = -0.0782$			
Optimum controller settings	K_c	0.150	0.120	0.115	0.064	0.00005
	τ_I	23.0	∞	100.0	10.0	1.0
X_D	M.D.	-9.98	-9.04	-9.14	-9.54	-6.97
	Off.	-6.88	-6.88	-6.88	-6.88	-6.88
	S.T.	93.	38.	39.	48.	55.
	I.S.E.	5158.	5563.	5626.	5701.	5253.
X_W	M.D.	4.32	1.63	1.63	1.75	2.09
	Off.	0.00	0.00	0.00	0.00	0.00
	S.T.	120.	67.	72.	88.	92.
	I.S.E.	159.9	17.48	18.64	35.32	52.47

Table 6.4-8

Feedback Control of the Liquid Composition on an Intermediate Tray

by Manipulation of Steam Flow

(University of Delaware Column)

Control Tray		1	3	7	9
Optimum controller settings	K_c	-0.375	-0.50	-1.60	-1.95
	τ_I	12.5	17.0	12.5	12.5
X_D	M.D.	-1.13	-3.64	-2.07	-1.09
	Off.	-0.61	-2.18	-0.97	0.28
	S.T.	65.	46.	39.	59.
	I.S.E.	38.30	570.5	145.8	16.30
X_W	M.D.	5.61	3.44	4.93	6.58
	Off.	5.39	3.31	4.93	6.58
	S.T.	34.	40.	36.	35.
	I.S.E.	3070.	1082.	2368.	8596.
X_i	M.D.	3.76	5.88	2.12	1.31
	Off.	0.00	0.00	0.00	0.00
	S.T.	84.	54.	23.	15.
	I.S.E.	64.21	117.3	6.803	2.739

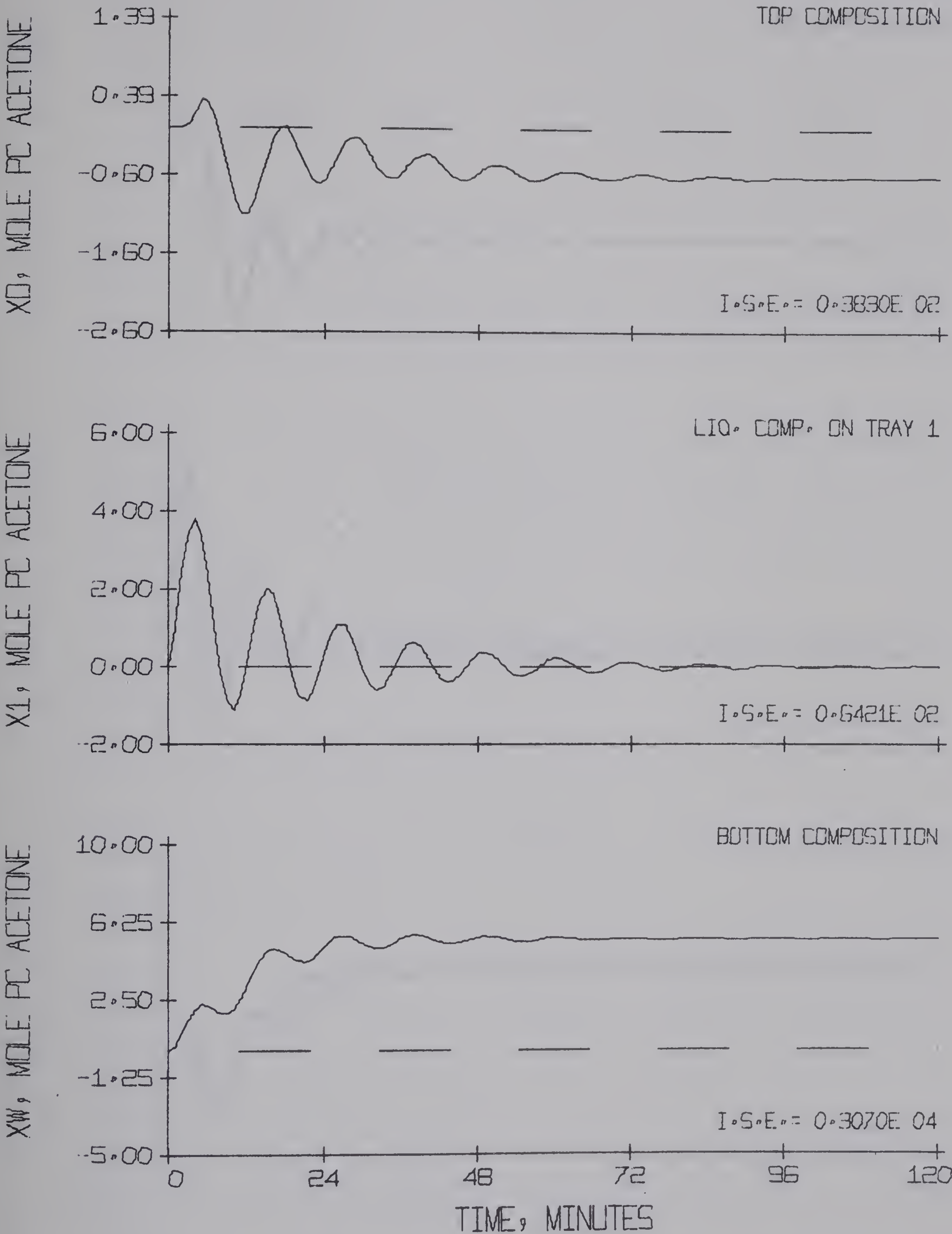
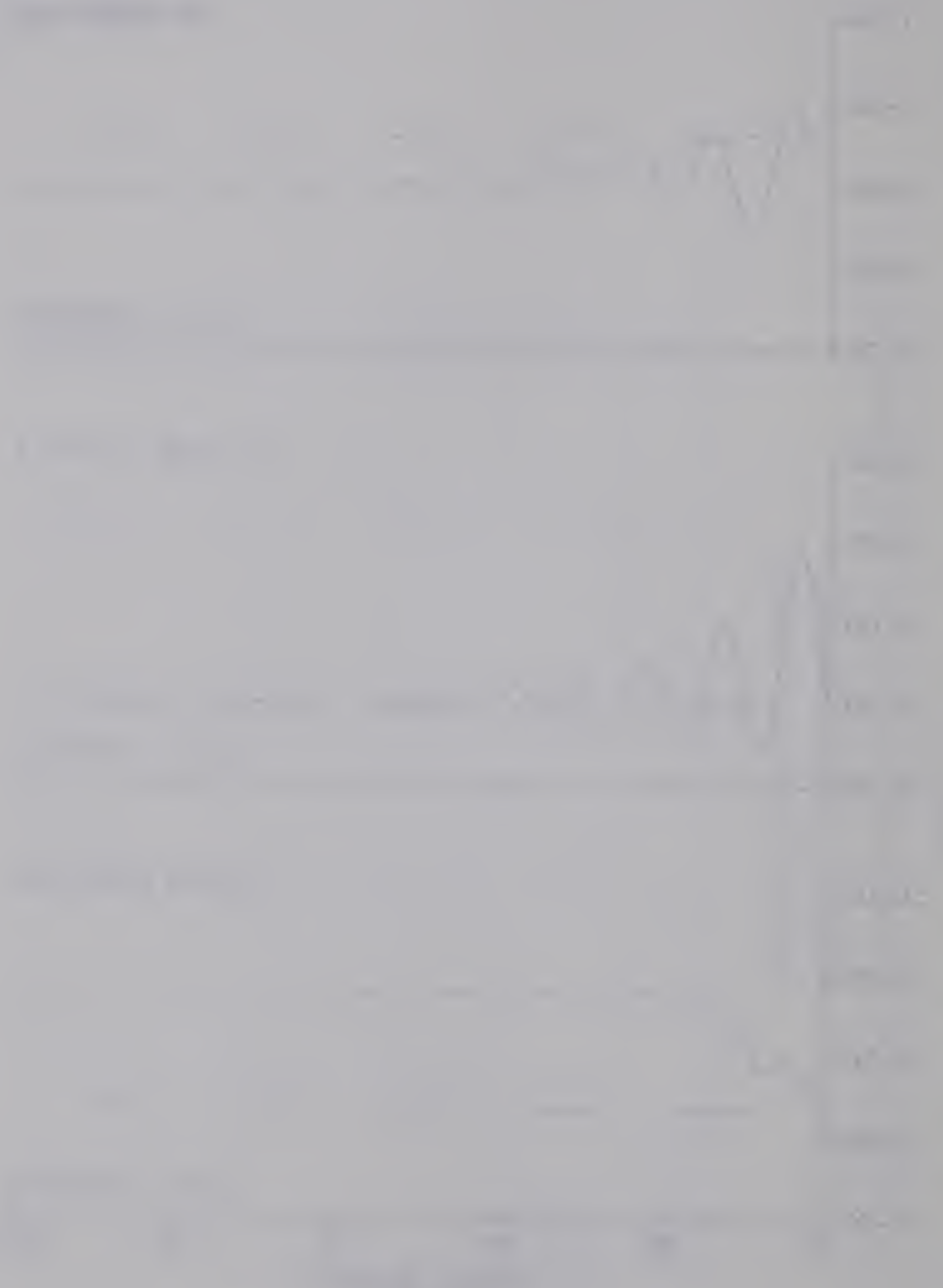


Figure 6.4-11 Feedback Control of the Liquid Composition on Tray 1
by Manipulation of Steam Flow
(University of Delaware Column)



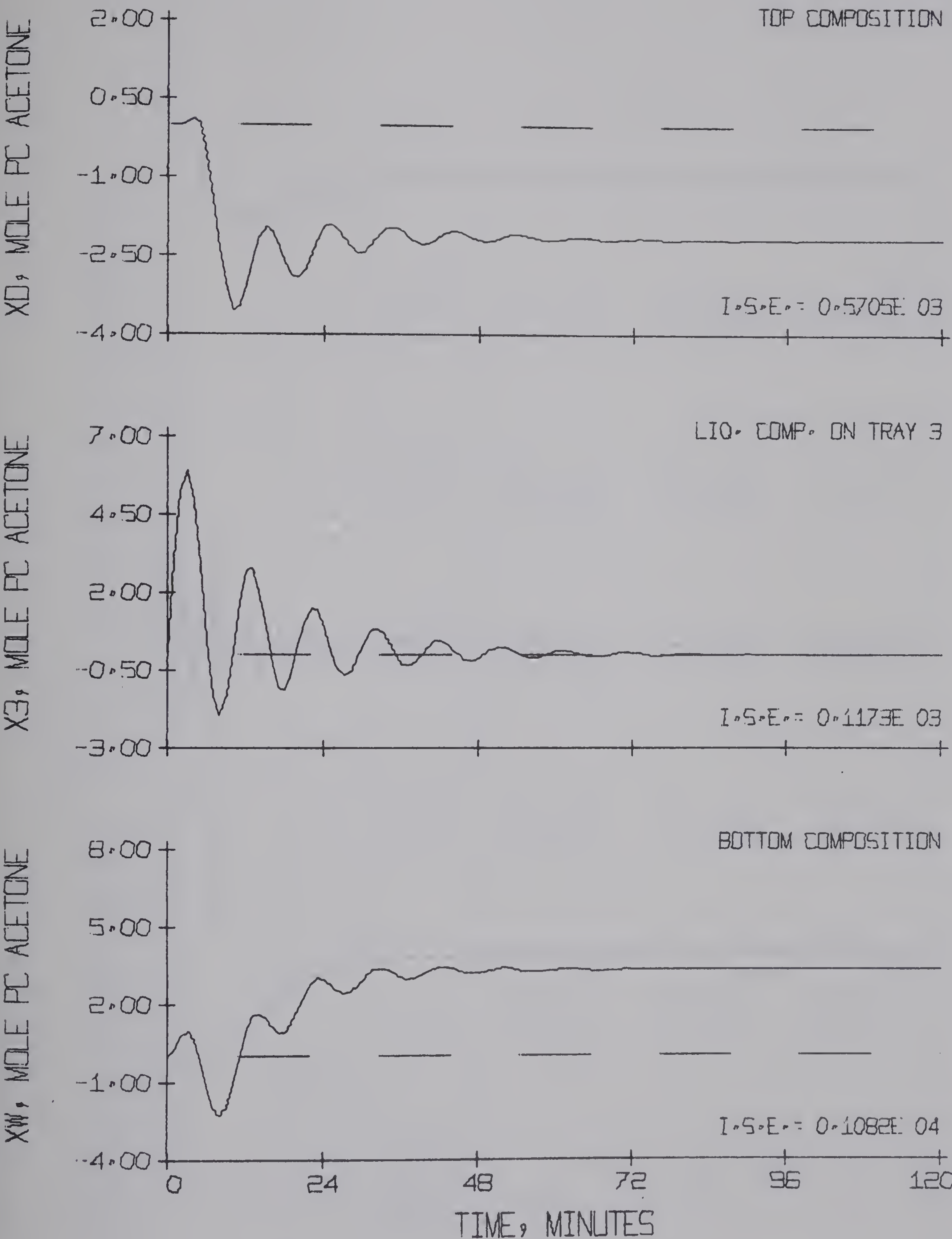


Figure 6.4-12 Feedback Control of the Liquid Composition on Tray 3 by Manipulation of Steam Flow (University of Delaware Column)

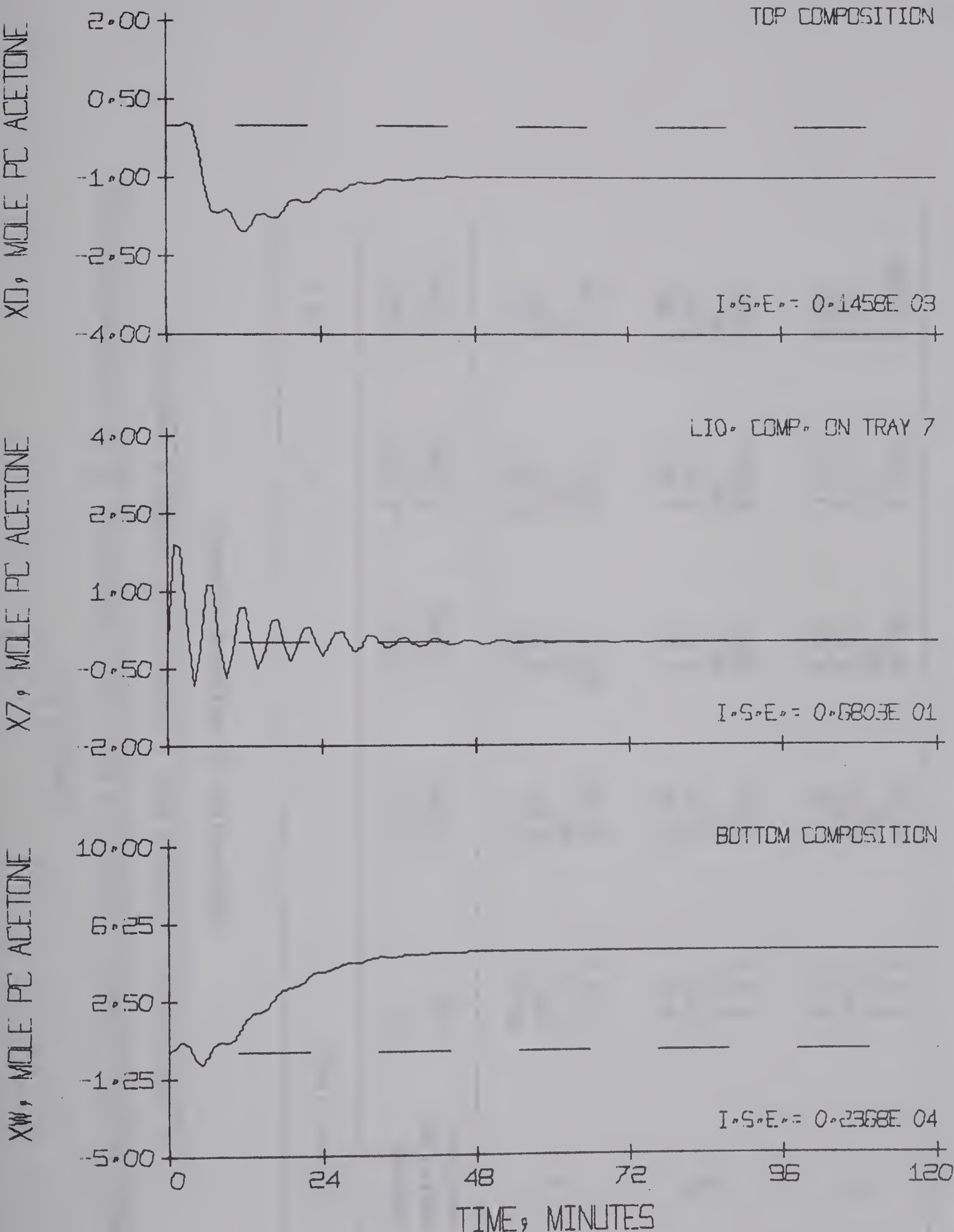


Figure 6.4-13 Feedback Control of the Liquid Composition on Tray 7 by Manipulation of Steam Flow (University of Delaware Column)

Table 6.4-9

Feedforward Plus Feedback Control of the Liquid Composition on an Intermediate Tray by Manipulation of Steam Flow - Proportional Feedback Controller

(University of Delaware Column)

Control Tray		1	3	7	9
Optimum controller settings	K_c	-0.061	-0.092	-0.337	-0.403
	K_{FF}	0.0061	0.0082	0.0065	0.0050
X_D	M.D.	-1.11	-3.52	-2.09	-1.10
	Off.	-0.61	-2.18	-0.97	0.28
	S.T.	55.	31.	39.	57.
	I.S.E.	42.47	602.1	149.3	17.36
X_W	M.D.	5.39	3.31	4.93	6.48
	Off.	5.39	3.31	4.93	6.58
	S.T.	26.	39.	36.	35.
	I.S.E.	3014.	1062.	2366.	4314.
X_i	M.D.	1.76	4.09	1.32	0.80
	Off.	0.00	0.00	0.00	0.00
	S.T.	34.	33.	14.	7.
	I.S.E.	9.54	44.46	2.038	0.7738

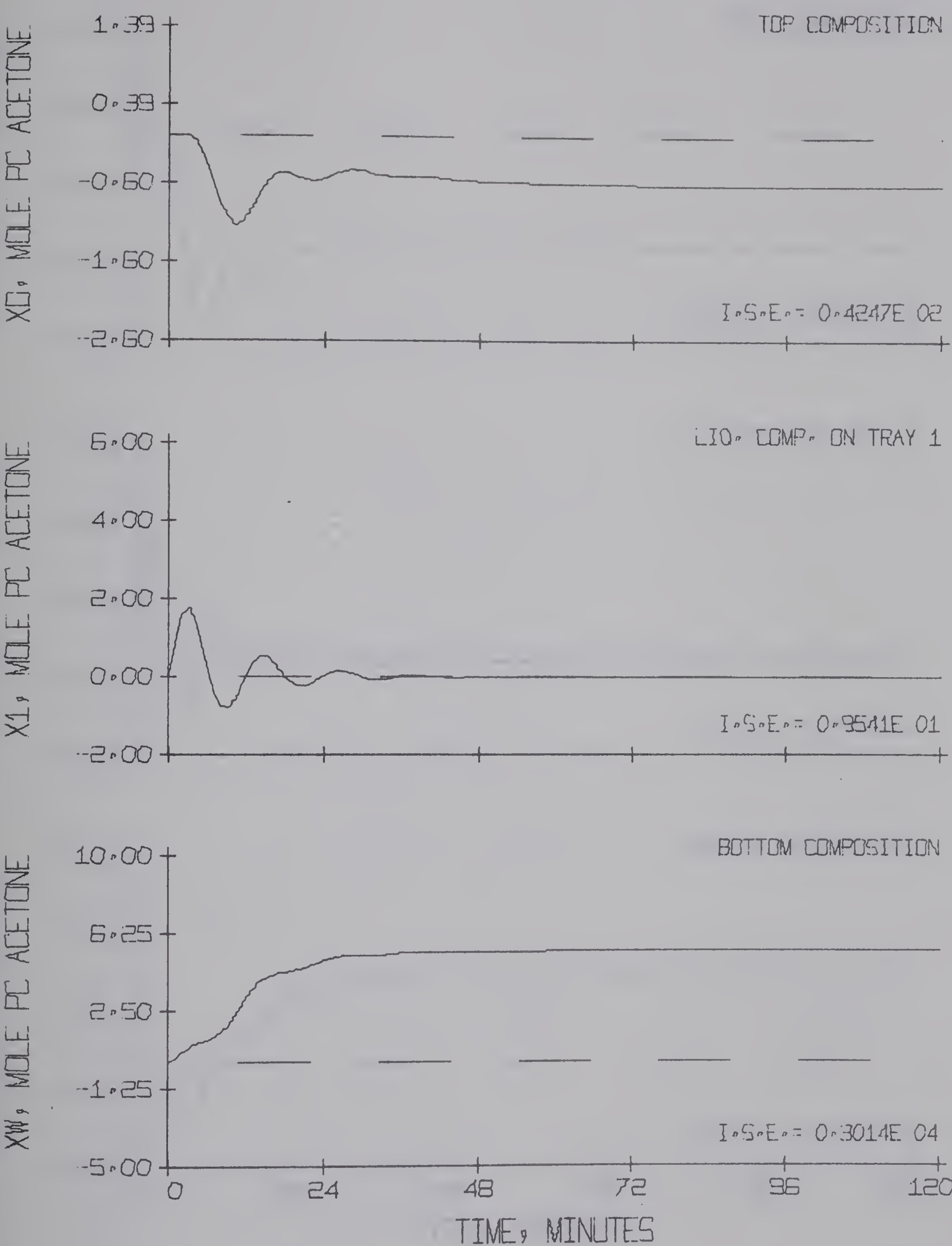


Figure 6.4-14 Feedforward Plus Feedback Control of the Liquid Composition on Tray 1 by Manipulation of Steam Flow - Proportional Feedback Controller (University of Delaware Column)

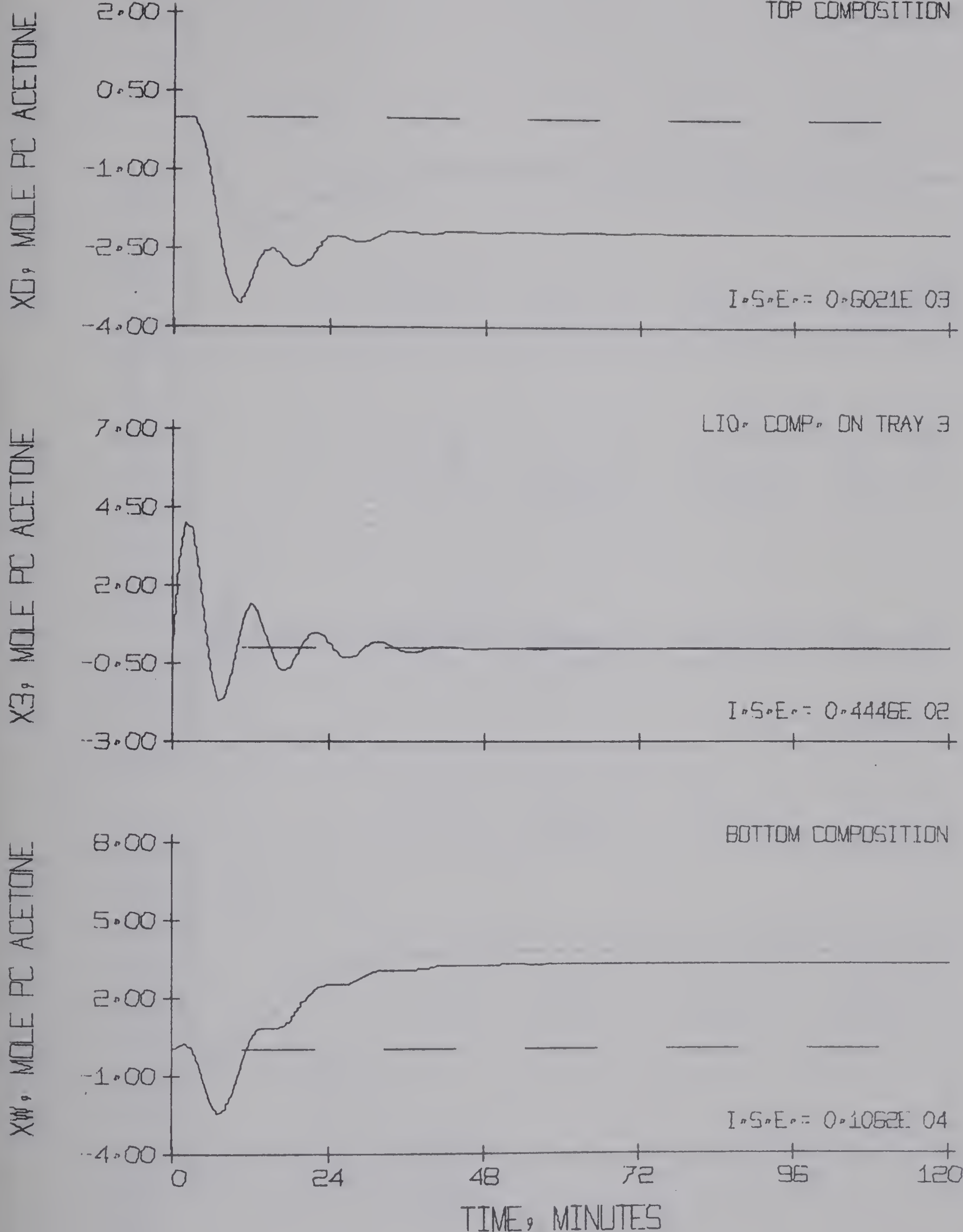
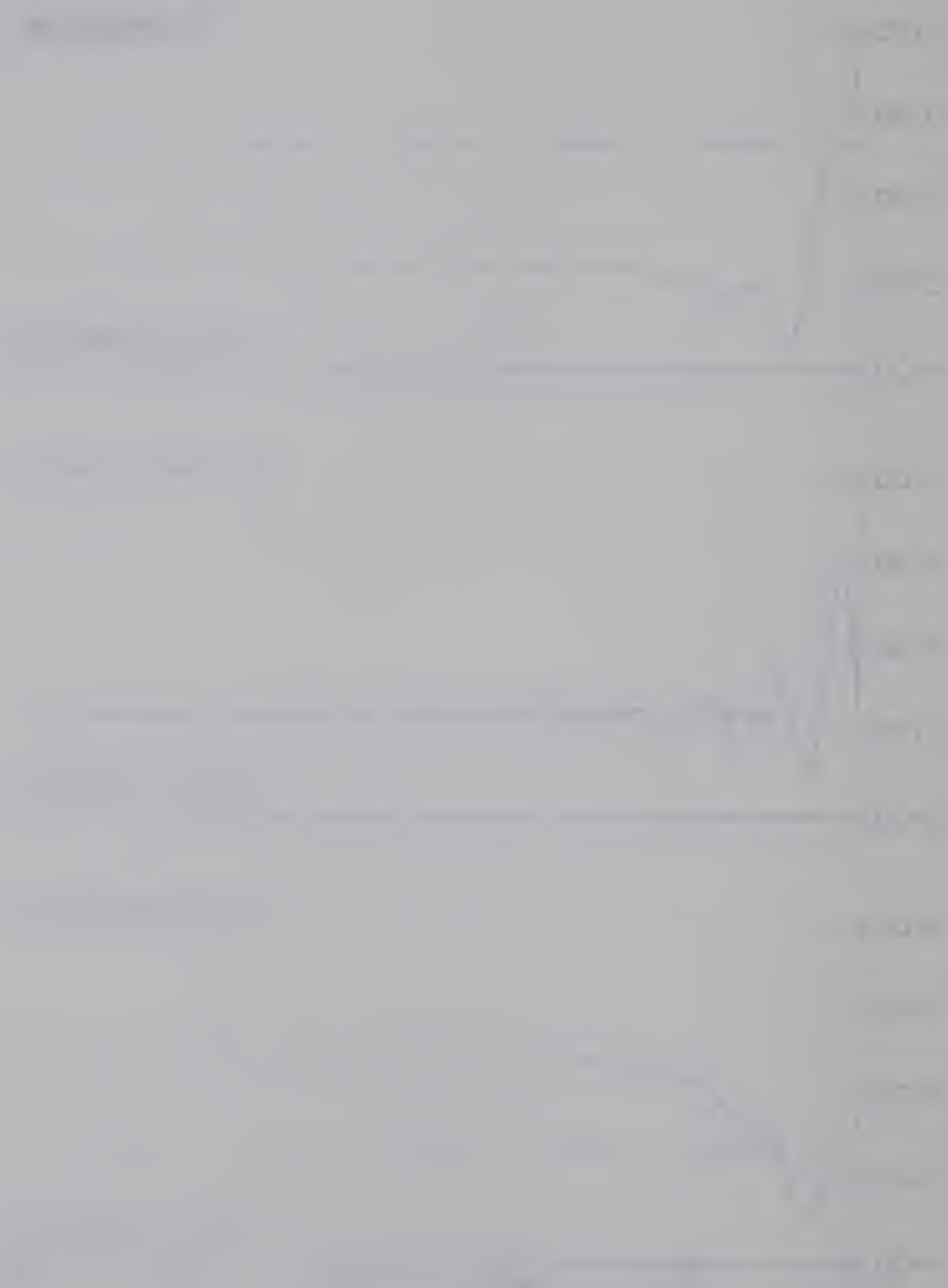


Figure 6.4-15 Feedforward Plus Feedback Control of the Liquid Composition on Tray 3 by Manipulation of Steam Flow - Proportional Feedback Controller (University of Delaware Column)



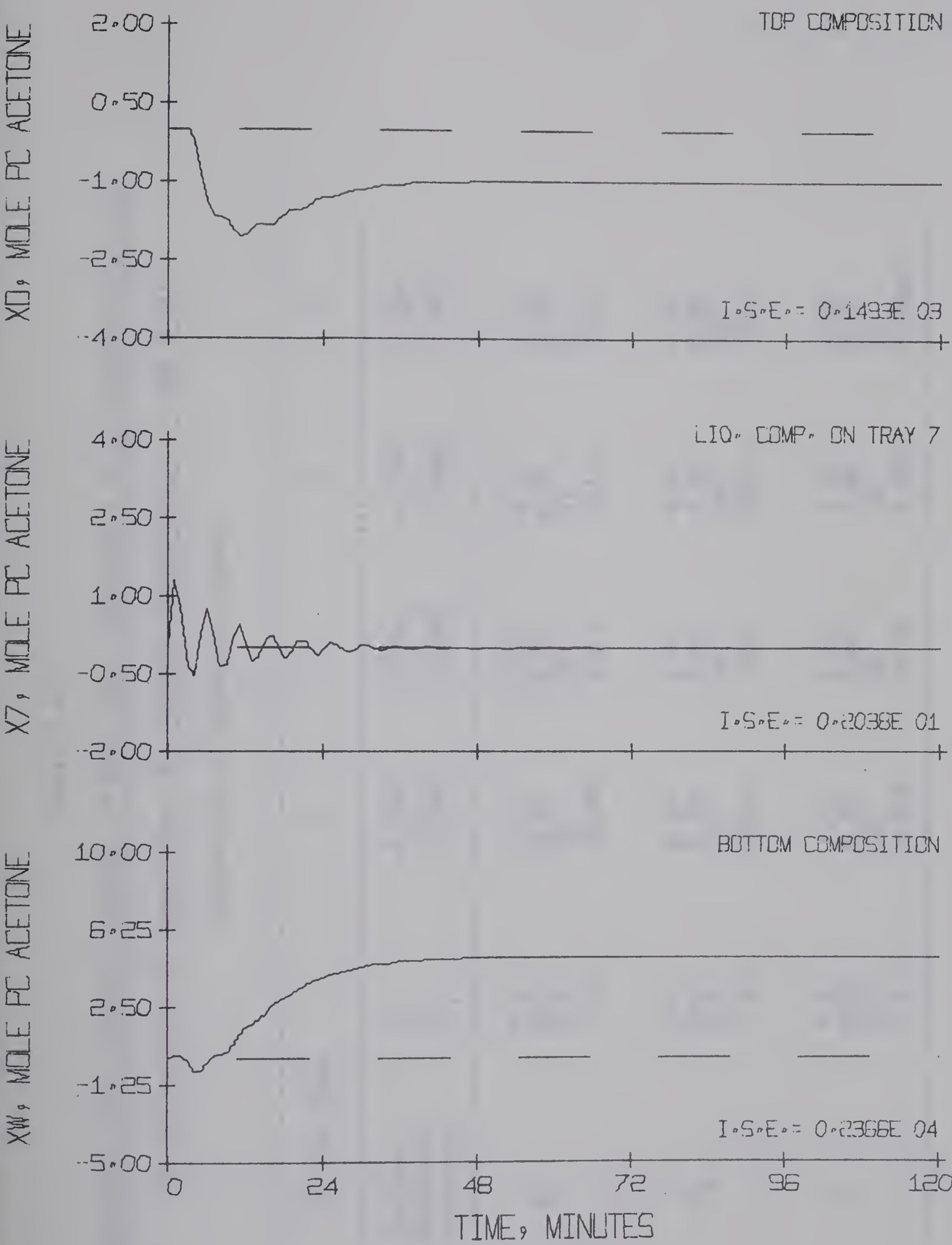


Figure 6.4-16 Feedforward Plus Feedback Control of the Liquid Composition on Tray 7 by Manipulation of Steam Flow - Proportional Feedback Controller (University of Delaware Column)

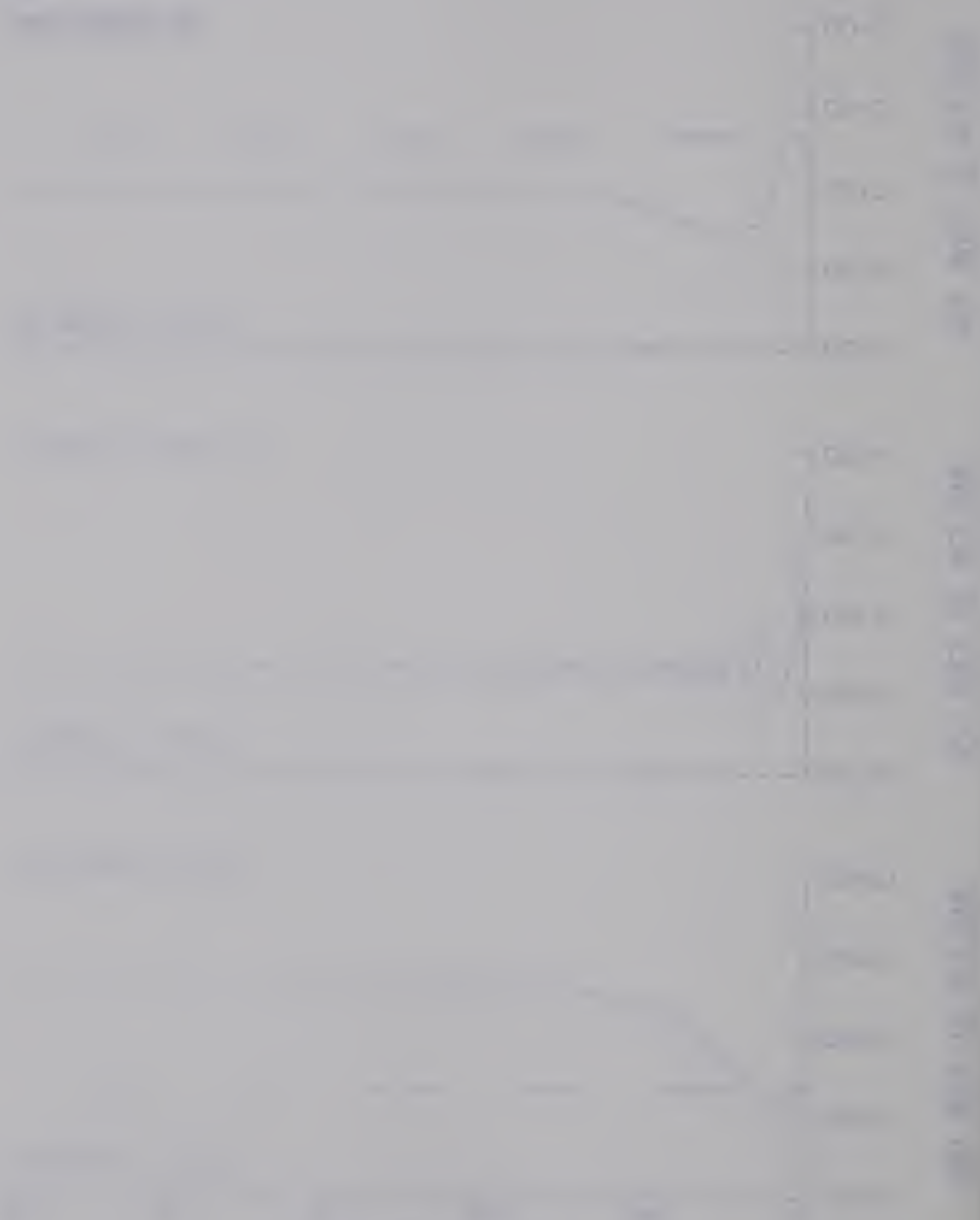


Table 6.4-10

Feedforward Plus Feedback Control of the Liquid Composition on an Intermediate Tray by Manipulation of Steam Flow - PI Feedback Controller, τ_I = 100.0 min.

(University of Delaware Column)

Control Tray		1	3	7	9
Optimum controller settings	K_c	-0.059	-0.090	-0.330	-0.399
	K_{FF}	0.0061	0.0082	0.0065	0.0050
X_D	M.D.	-1.12	-3.56	-2.07	-1.11
	Off.	-0.62	-2.19	-0.97	0.28
	S.T.	52.	32.	41.	61.
	I.S.E.	43.88	616.6	151.2	17.33
X_W	M.D.	5.39	3.30	4.93	6.58
	Off.	5.39	3.30	4.93	6.58
	S.T.	27.	40.	36.	35.
	I.S.E.	2998.	1040.	2357.	4304.
X_i	M.D.	1.72	4.10	1.32	0.80
	Off.	0.00	0.00	0.00	0.00
	S.T.	36.	39.	14.	7.
	I.S.E.	9.862	45.76	2.064	0.7800

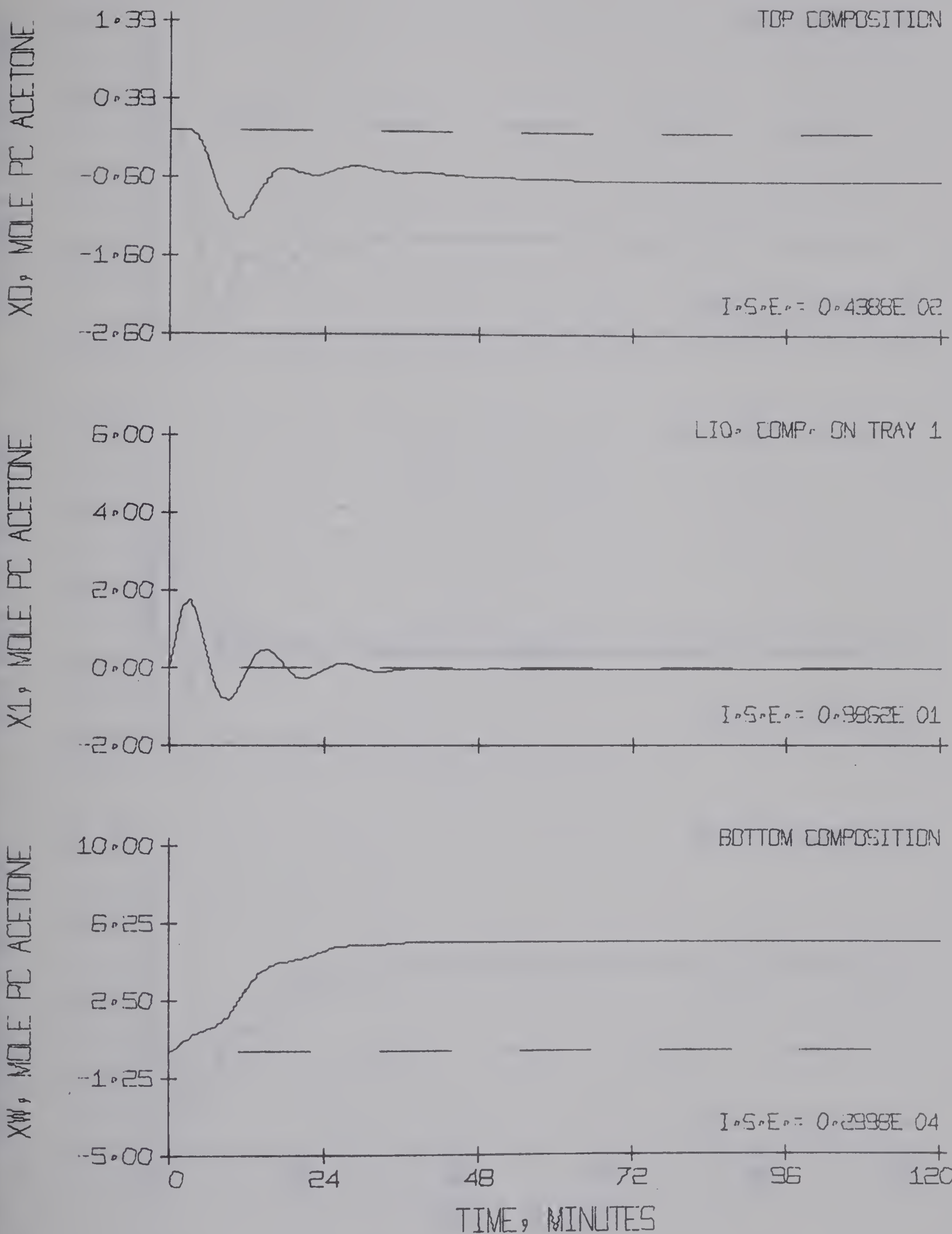
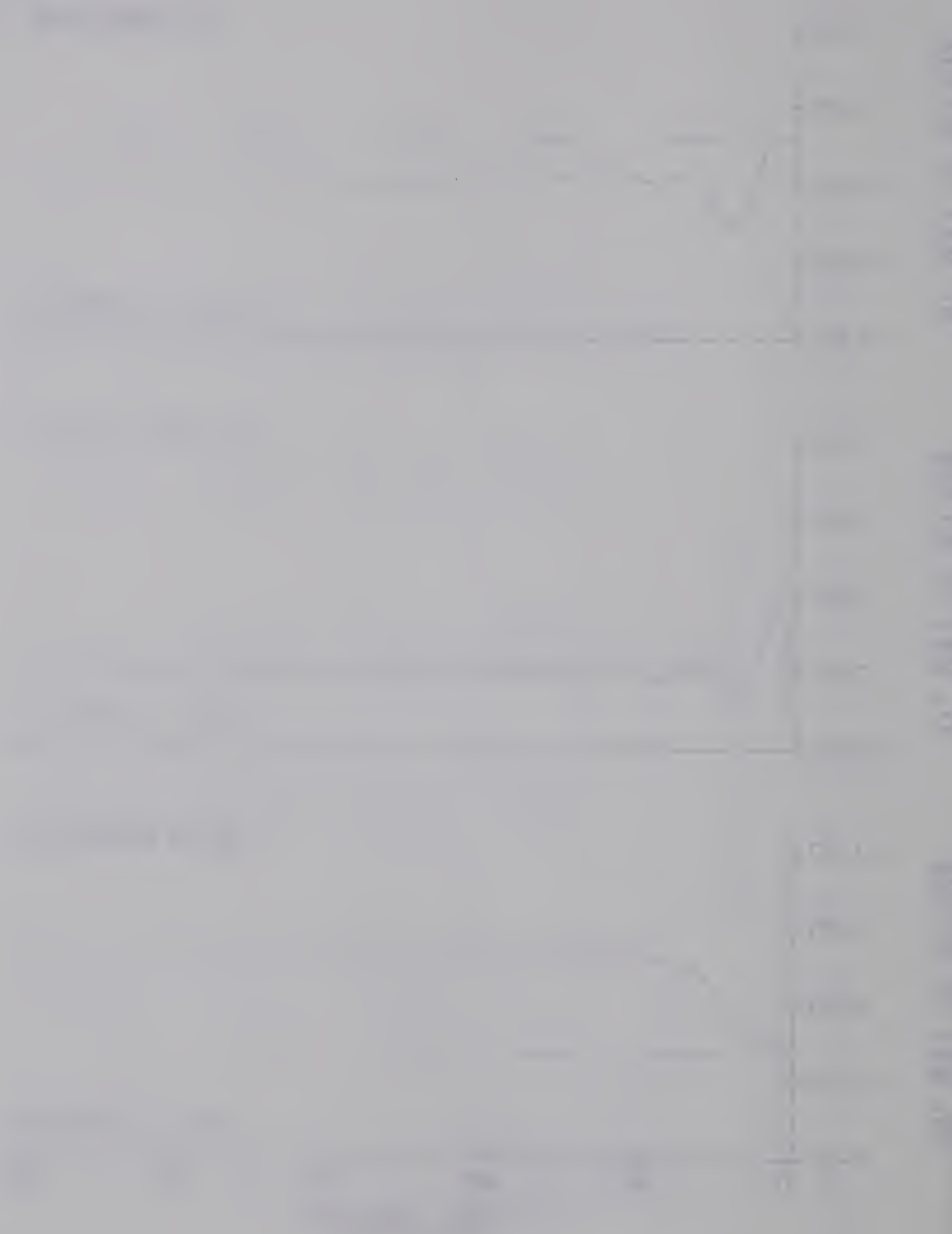


Figure 6.4-17 Feedforward Plus Feedback Control of the Liquid Composition on Tray 1 by Manipulation of Steam Flow - PI Feedback Controller, τ_I = 100.0 min. (University of Delaware Column)



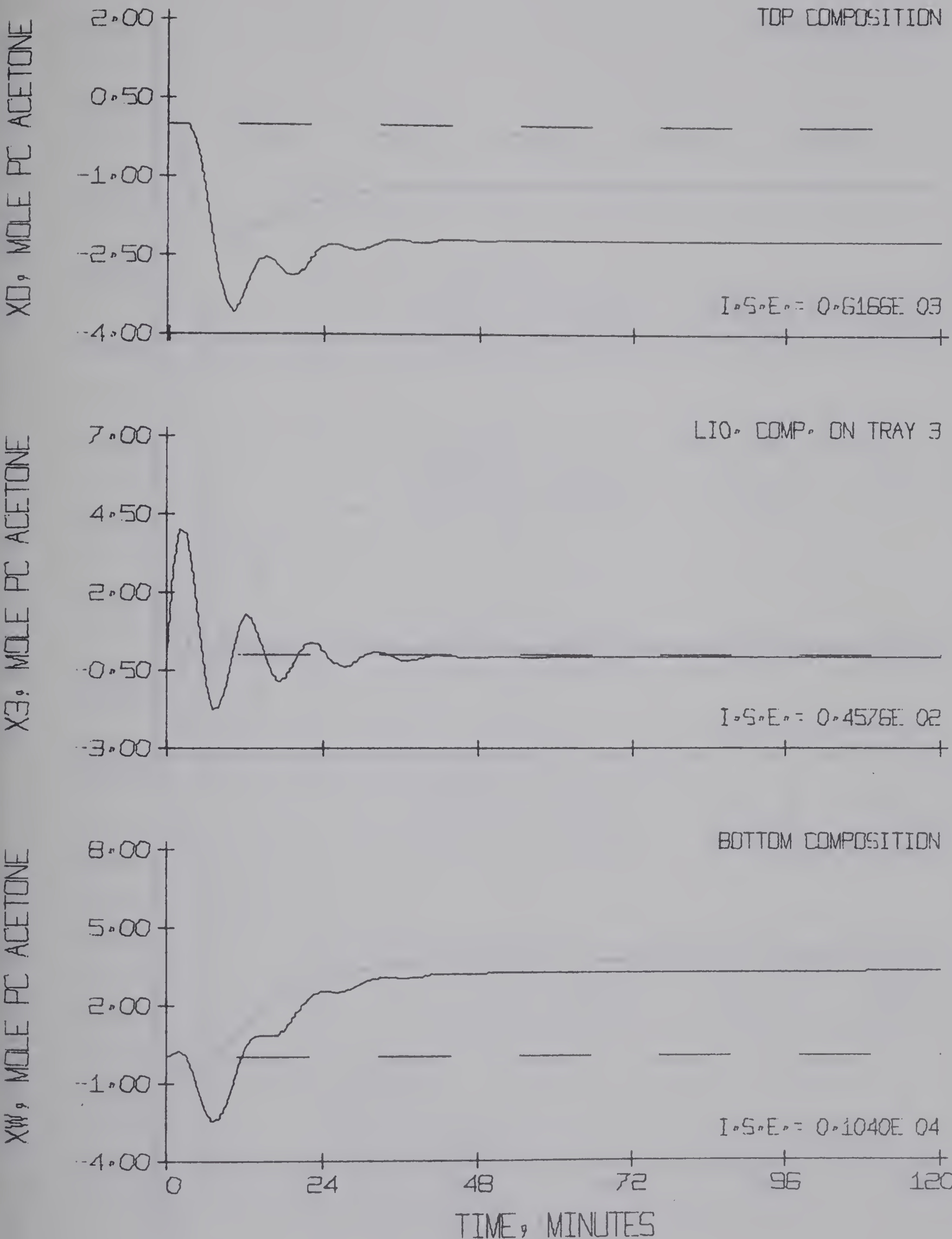
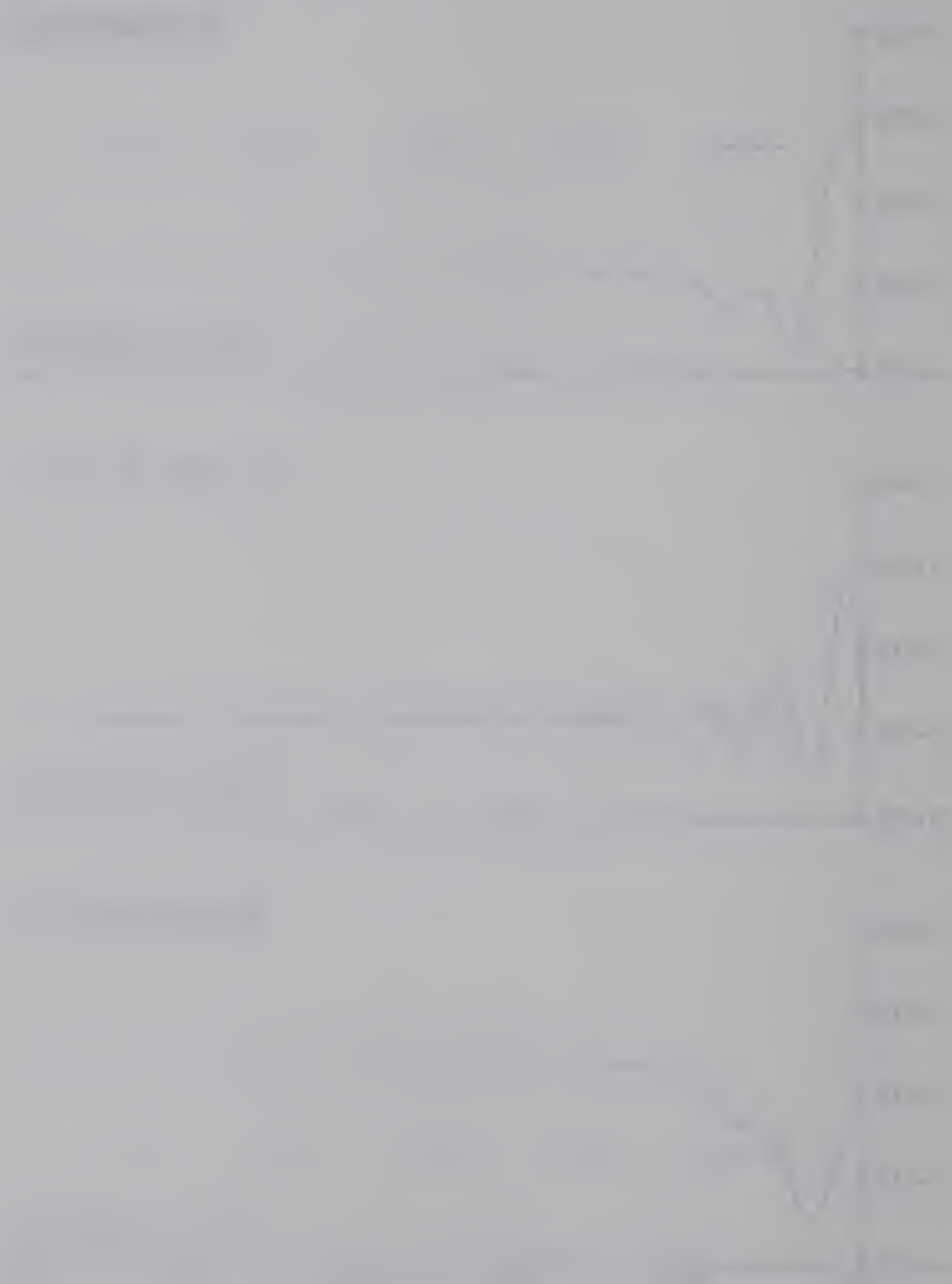


Figure 6.4-18 Feedforward Plus Feedback Control of the Liquid Composition on Tray 3 by Manipulation of Steam Flow - PI Feedback Controller, τ_I = 100.0 min. (University of Delaware Column)



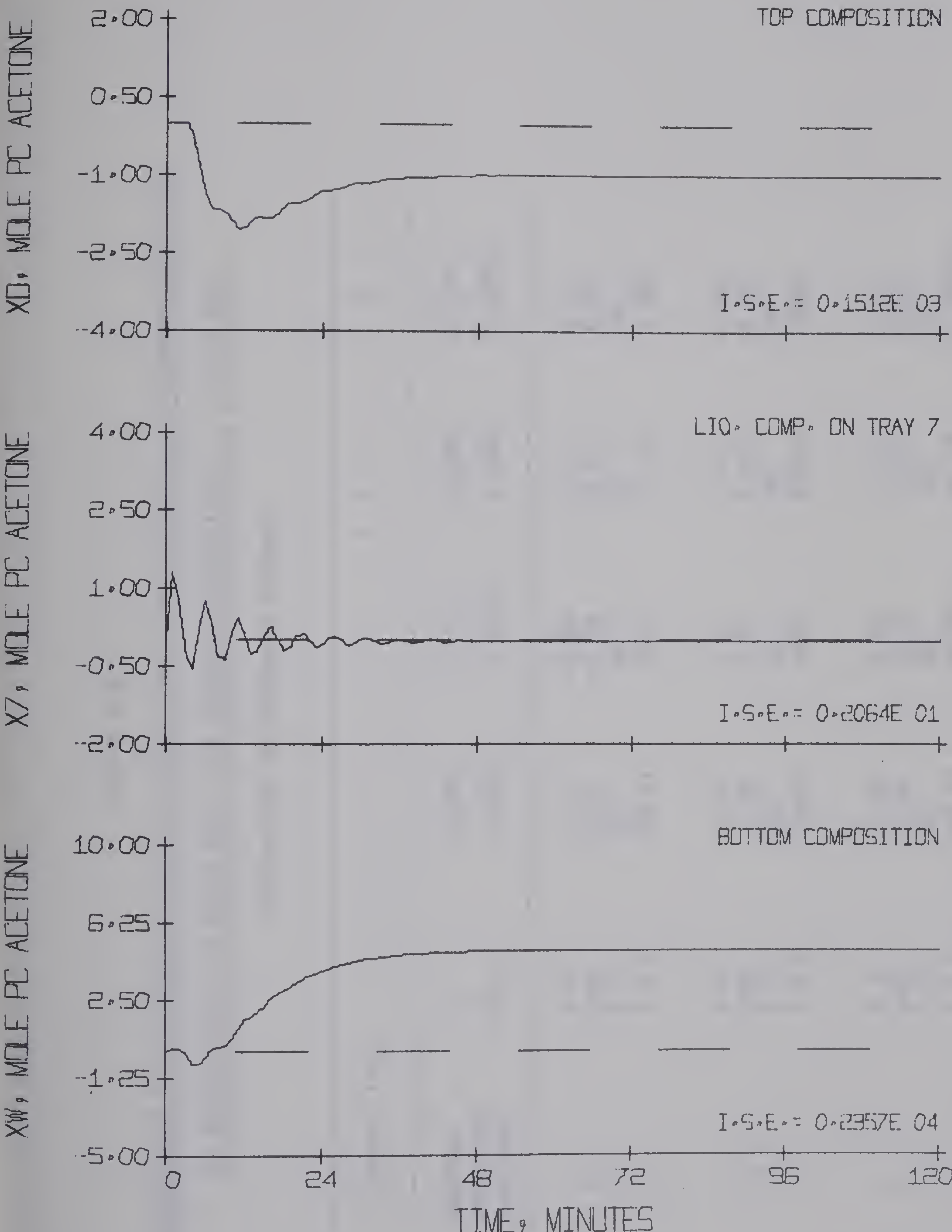


Figure 6.4-19 Feedforward Plus Feedback Control of the Liquid Composition on Tray 7 by Manipulation of Steam Flow - PI Feedback Controller, τ_I = 100.0 min. (University of Delaware Column)

Table 6.4-11

Feedforward Plus Feedback Control of the Liquid Composition on an Intermediate Tray by Manipulation of Steam Flow - PI Feedback Controller, τ_I = 10.0 min.

(University of Delaware Column)

Control Tray		1	3	7	9
Optimum controller settings	K_c	-0.046	-0.074	-0.280	-0.336
	K_{FF}	0.0061	0.0082	0.0065	0.0050
X_D	M.D.	-1.21	-3.94	-2.13	-1.12
	Off.	-0.61	-2.18	-0.97	0.28
	S.T.	52.	36.	41.	58.
	I.S.E.	45.41	63.17	15.35	1.850
X_W	M.D.	5.39	3.31	4.93	6.58
	Off.	5.39	3.31	4.93	6.58
	S.T.	29.	36.	36.	34.
	I.S.E.	2995.	1063.	2360.	4305.
X_i	M.D.	1.80	4.17	1.33	0.81
	Off.	0.00	0.00	0.00	0.00
	S.T.	41.	34.	16.	10.
	I.S.E.	14.13	63.56	25.19	0.9330

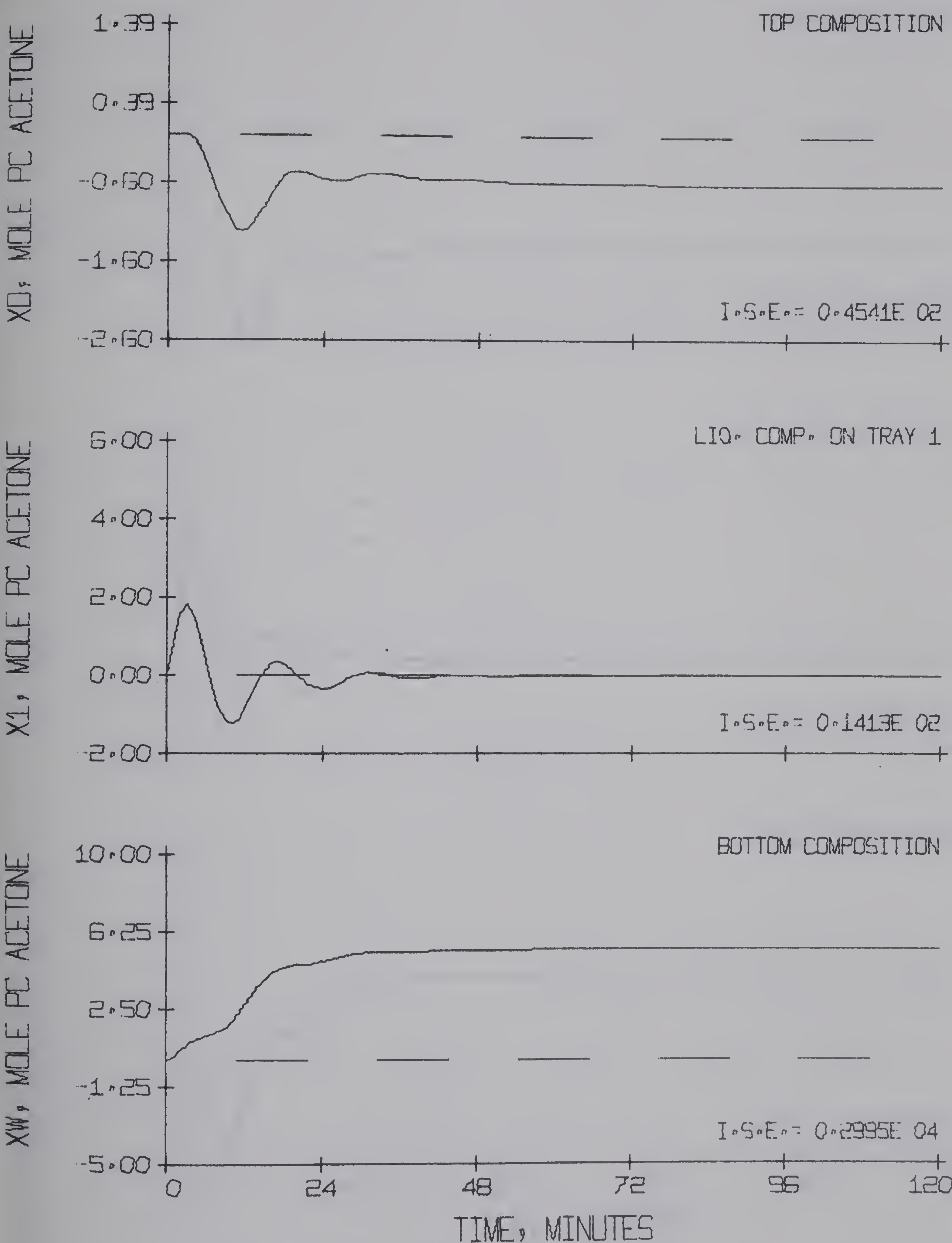
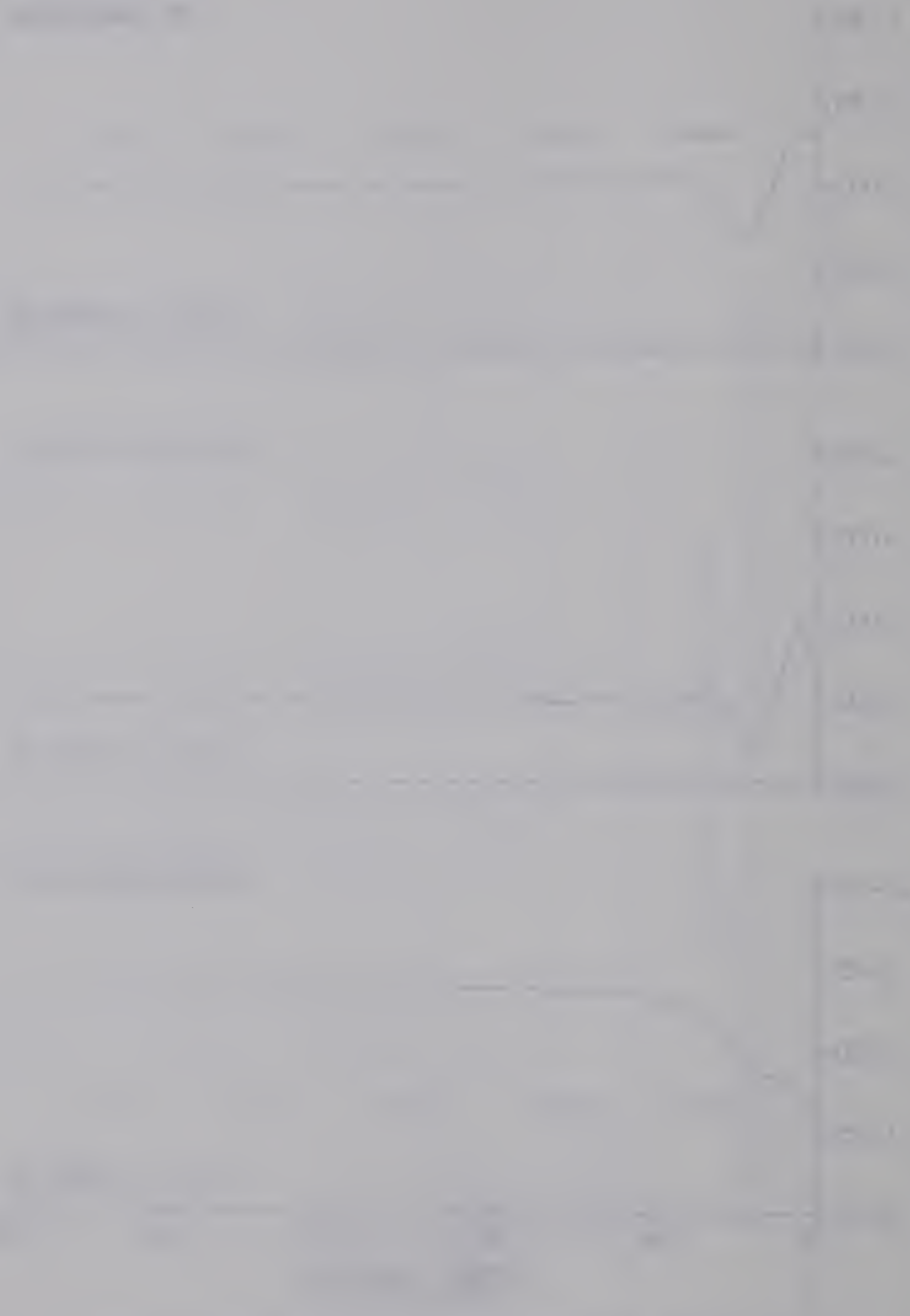


Figure 6.4-20 Feedforward plus Feedback Control of the Liquid Composition on Tray 1 by Manipulation of Steam Flow - PI Feedback Controller, τ_I = 10.0 min. (University of Delaware Column)



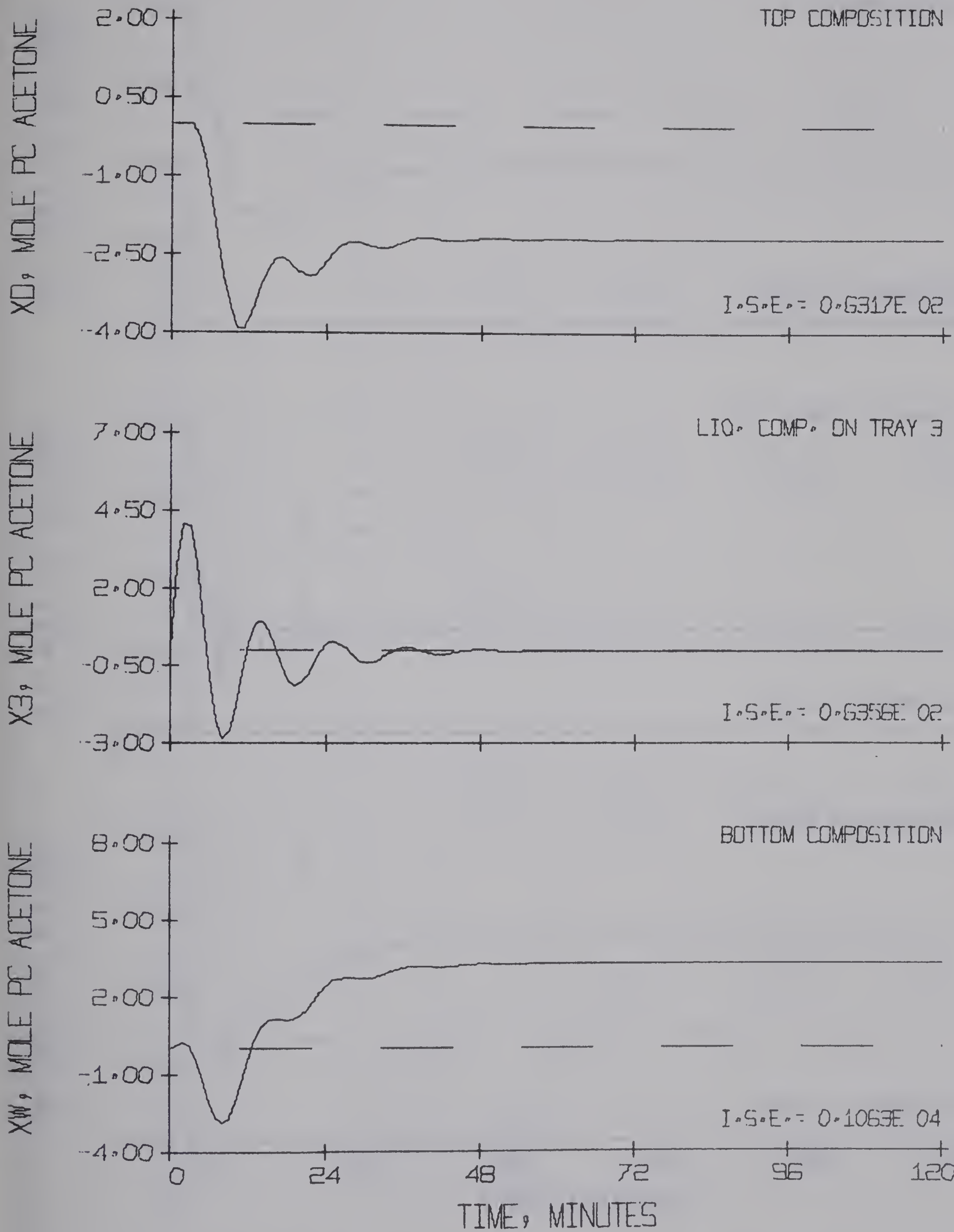
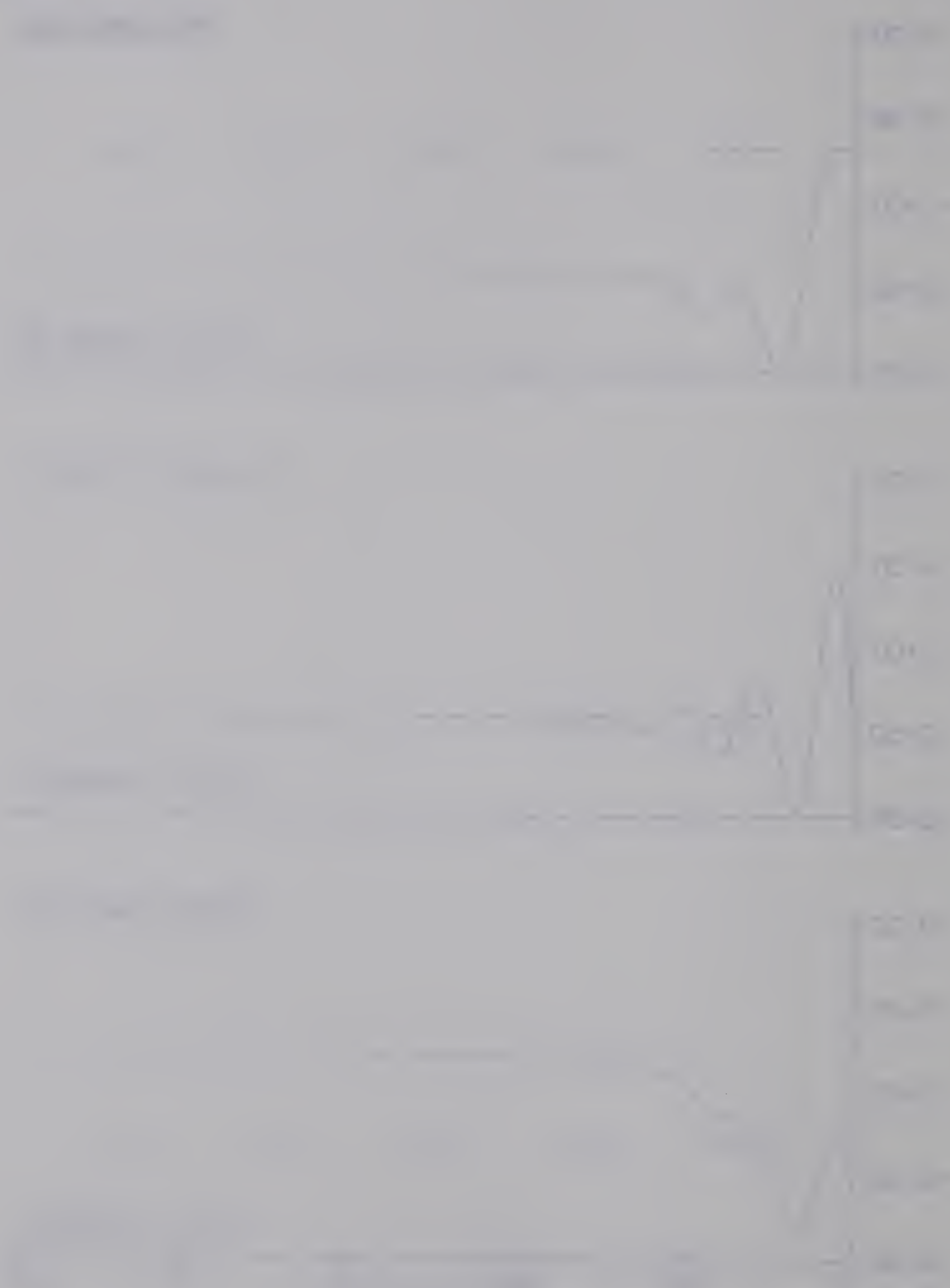


Figure 6.4-21 Feedforward Plus Feedback Control of the Liquid Composition on Tray 3 by Manipulation of Steam Flow - PI Feedback Controller, τ_I = 10.0 min. (University of Delaware Column)



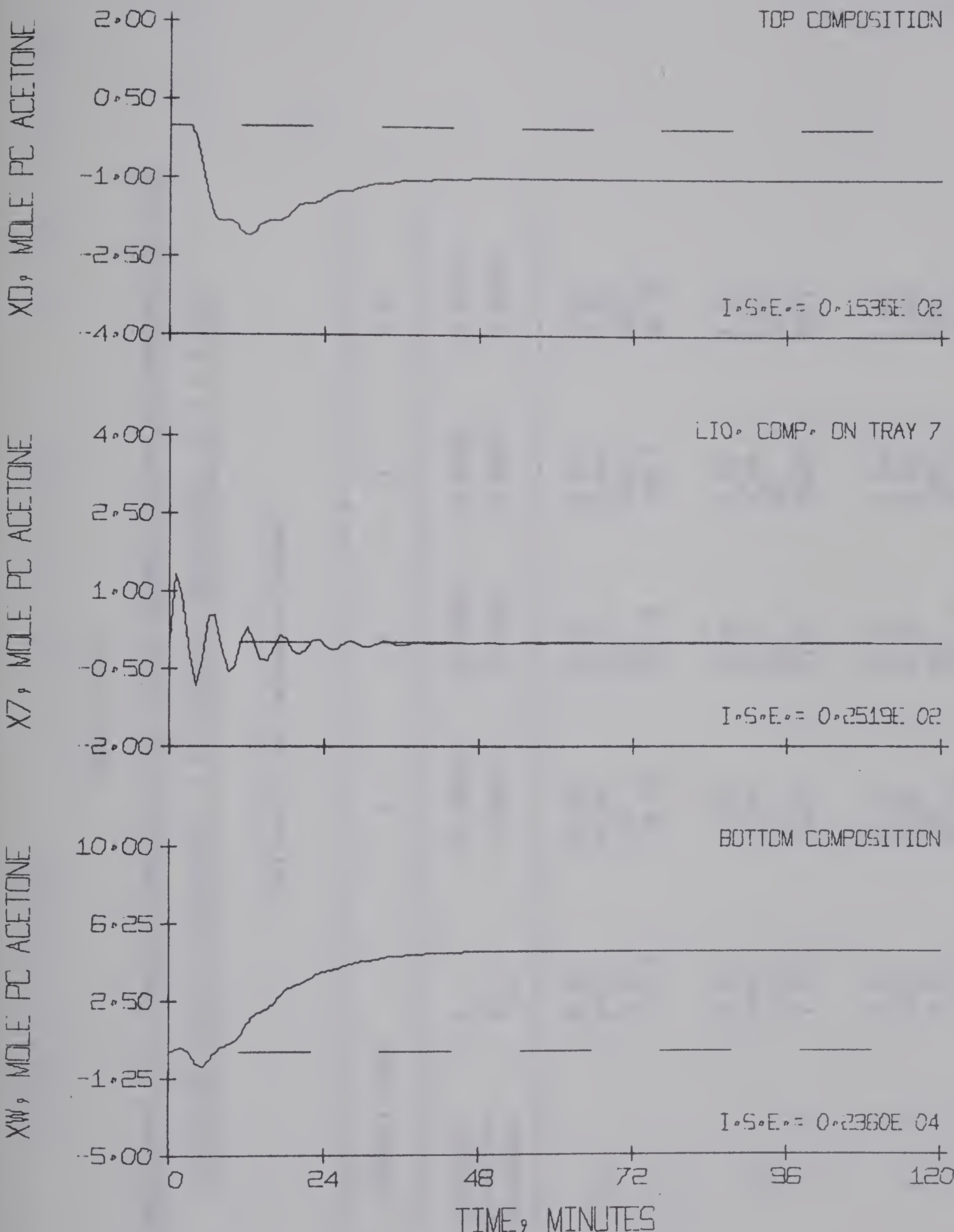


Figure 6.4-22 Feedforward Plus Feedback Control of the Liquid Composition on Tray 7 by Manipulation of Steam Flow - PI Feedback Controller, τ_I = 10.0 min. (University of Delaware Column)

Table 6.4-12

Feedforward Plus Feedback Control of the Liquid Composition on an Intermediate Tray by Manipulation of Steam Flow - PI Feedback Controller, τ_I = 1.0 min.

(University of Delaware Column)

Control Tray		1	3	7	9
Optimum controller settings	K_c	-0.00003	-0.00003	-0.0098	-0.0112
	K_{FF}	0.0061	0.0082	0.0065	0.0050
X_D	M.D.	-0.65	-2.28	-2.91	-1.52
	Off.	-0.64	-2.26	-0.96	0.28
	S.T.	78.	82.	120.	120.
	I.S.E.	34.70	487.8	180.2	32.52
X_W	M.D.	5.37	3.25	5.79	7.19
	Off.	5.36	3.21	4.94	6.58
	S.T.	41.	43.	80.	72.
	I.S.E.	3069.	1102.	2389.	4311.
X_i	M.D.	2.16	5.81	-2.93	-1.88
	Off.	0.00	0.00	0.00	0.00
	S.T.	36.	42.	120.	120.
	I.S.E.	47.48	411.7	123.4	56.47

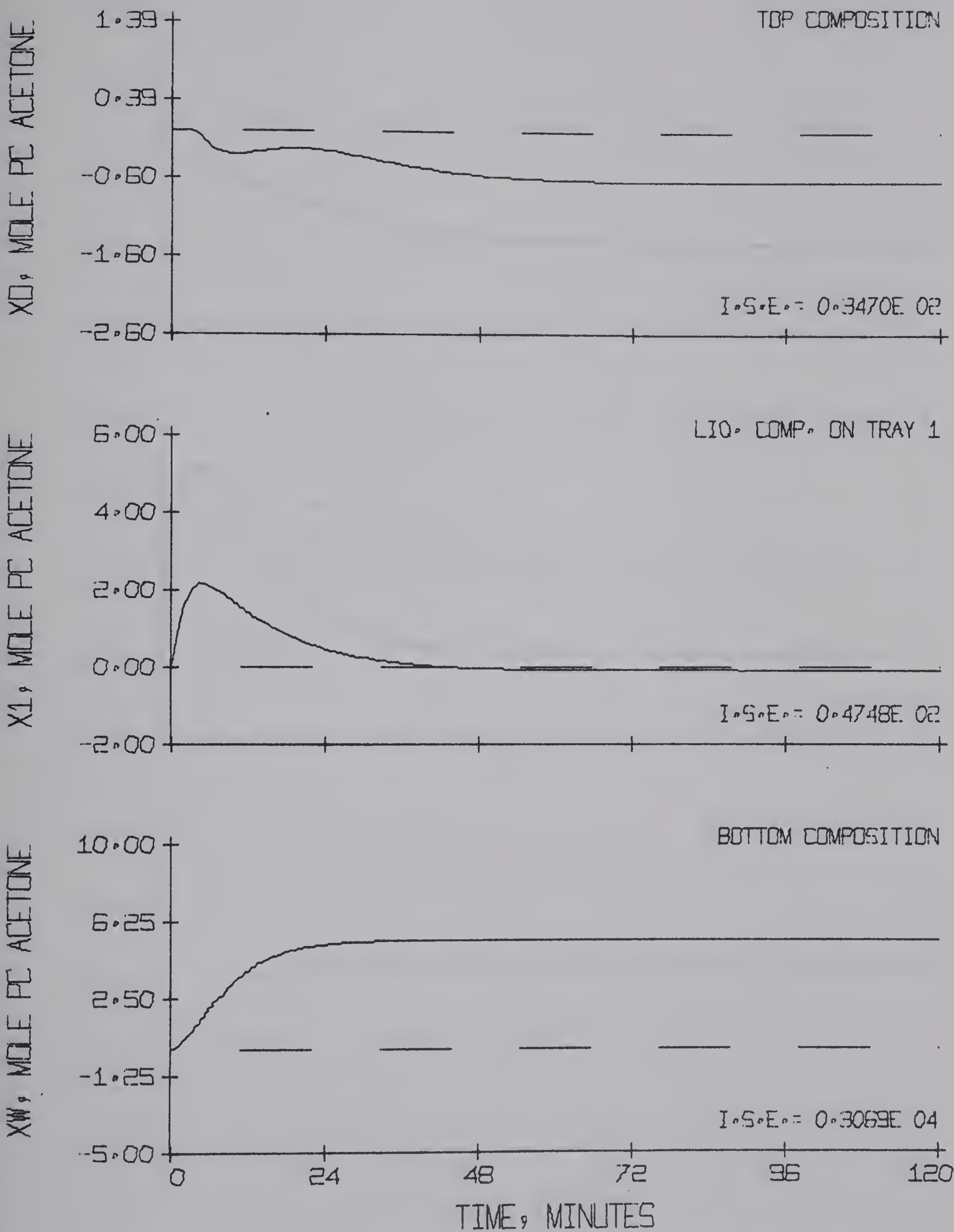


Figure 6.4-23 Feedforward Plus Feedback Control of the Liquid Composition on Tray 1 by Manipulation of Steam Flow - PI Feedback Controller, τ_I = 1.0 min. (University of Delaware Column)

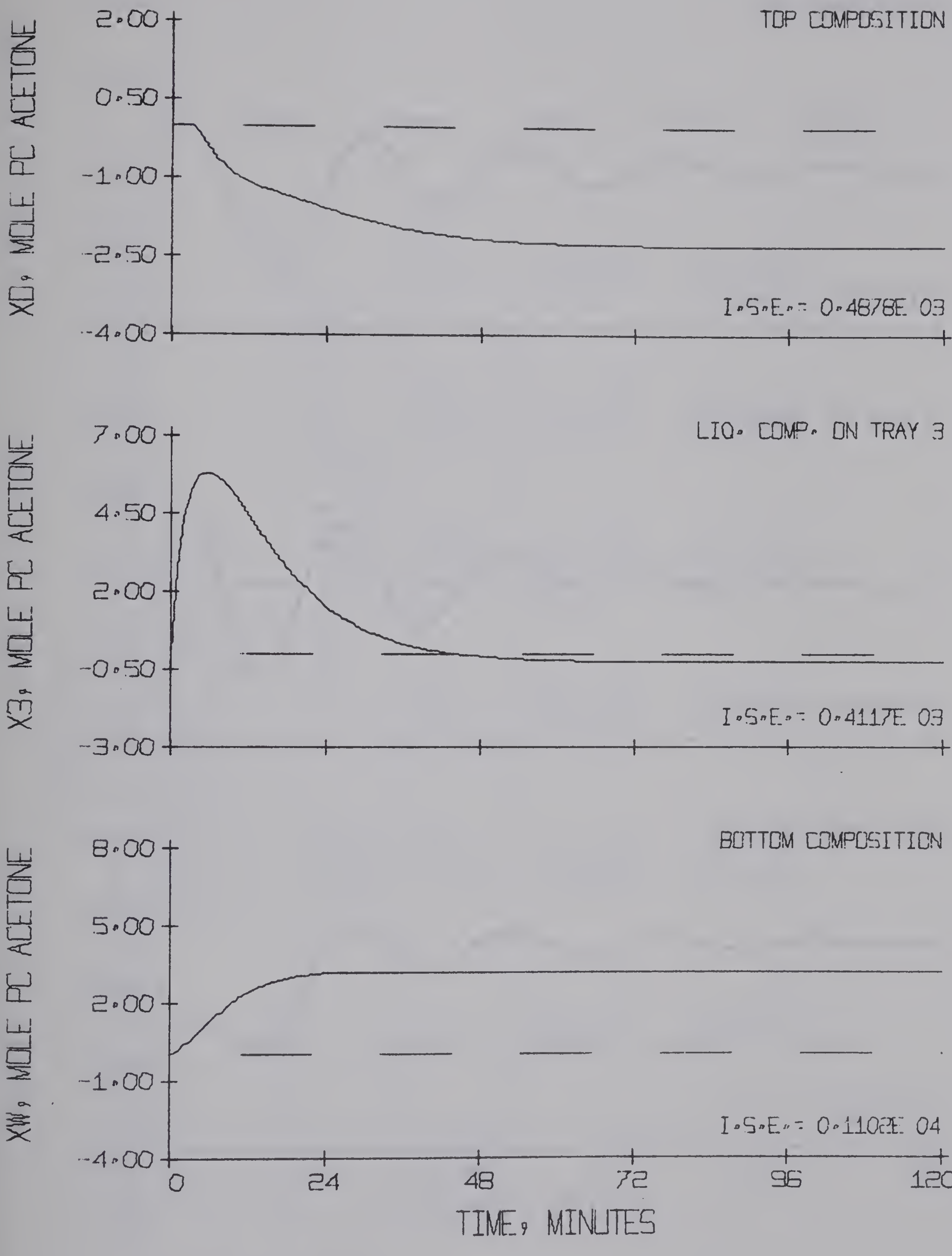


Figure 6.4-24 Feedforward Plus Feedback Control of the Liquid Composition on Tray 3 by Manipulation of Steam Flow - PI Feedback Controller, τ_I = 1.0 min. (University of Delaware Column)

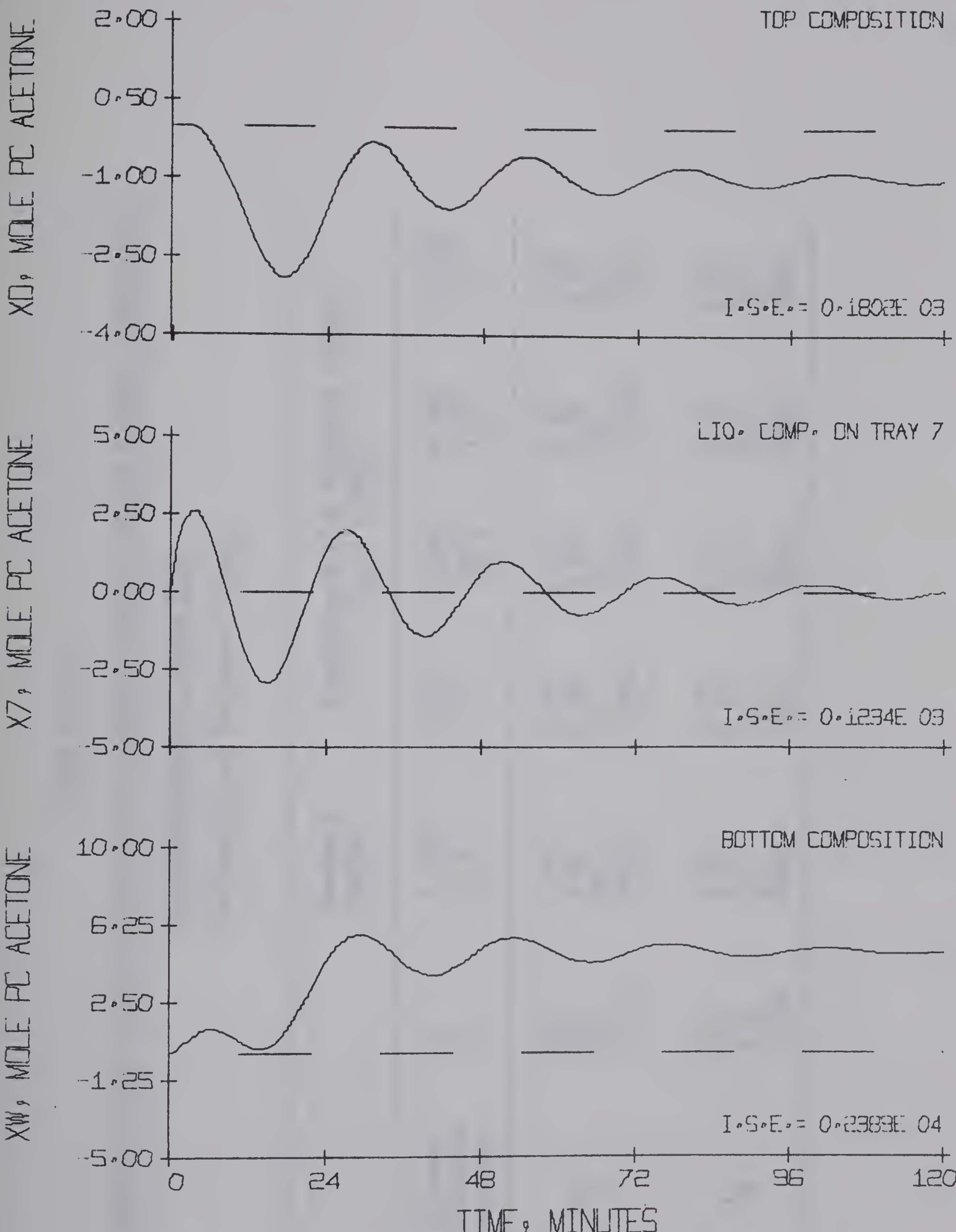


Figure 6.4-25 Feedforward Plus Feedback Control of the Liquid Composition on Tray 7 by Manipulation of Steam Flow - PI Feedback Controller, τ_I = 1.0 min. (University of Delaware Column)

Table 6.4-13

Feedback Control and Feedforward Plus Feedback Control of Top Product Composition

by Manipulation of Steam Flow

(University of Delaware Column)

		Feedback Control	Feedforward plus Feedback Control $K_{FF} = 0.0053$			
Optimum controller settings	K_c	-0.105	-0.093	-0.085	-0.062	-0.0006
	τ_I	16.0	∞	100.0	10.0	1.0
X_D	M.D.	1.70	0.25	0.25	0.27	0.28
	Off.	0.00	0.00	0.00	0.00	0.00
	S.T.	36.	10.	10.	10.	10.
	I.S.E.	24.02	0.4256	0.4444	0.7505	1.410
X_W	M.D.	6.82	6.21	6.21	6.21	6.21
	Off.	6.21	6.21	6.21	6.21	6.21
	S.T.	61.	32.	32.	37.	32.
	I.S.E.	4269.	4033.	4020.	4008.	4096.

Table 6.4-14

Feedback Control and Feedforward Plus Feedback Control of Bottom Product Composition by Manipulation of Steam Flow

(University of Delaware Column)

		Feedback Control	Feedforward plus Feedback Control $K_{FF} = 0.0107$			
Optimum controller settings	K_c	-0.145	-0.092	-0.087	-0.063	-0.0084
	τ_I	12.7	∞	100.0	10.0	1.0
X_D	M.D.	-4.77	-4.68	-4.68	-4.68	-4.71
	Off.	-4.68	-4.68	-4.68	-4.68	-4.68
	S.T.	58.	43.	42.	41.	48.
	I.S.E.	1978.	2145.	2149.	2152.	2152.
X_W	M.D.	2.59	0.18	0.18	0.18	0.18
	Off.	0.00	0.00	0.00	0.00	0.00
	S.T.	120.	18.	18.	19.	19.
	I.S.E.	38.03	0.1200	0.1174	0.1215	0.3757

In determining the dynamics of the measuring elements, it was found that all the thermocouples which were used to measure the temperature and the capacitance cell which was used to analyze top product composition have very rapid responses. Consequently, no dynamic lag is assigned to these measuring elements and the transfer functions H_D and H_i are considered to be unity. However, the dynamics for the analysis of the bottom product composition by means of the gas chromatograph are significant and must be considered. The bottom is sampled every 2.5 minutes by the gas chromatograph since a time of 2.5 minutes is required for analysis of the sample. This operation then would be rigorously represented by a time delay in series with a zero-order hold device. In order to simplify the simulations, it was assumed that the effects of intermittent sampling could be neglected so the transfer function representation for the gas chromatograph was taken as:

$$H_W = e^{-2.5s}$$

As was the case for the simulations done using data from the University of Delaware distillation column, the dynamics of the control valve were considered to be negligible.

A stepwise variation in feed flow rate of 0.430 lb./min. was used as the forcing function. This amount represents a change in feed flow rate from 50 per cent to 70 per cent on the feed flow recording chart. Only the results obtained using controller settings

which resulted in a minimum I.S.E. value in the controlled variable are presented herein. Furthermore, because of the large number of possible systems simulated, only some of the column responses to illustrate the general behavior are included. Those tests selected were the control of the liquid temperature on trays 6, 7, 8 by manipulation of reflux flow and the control of the liquid temperature on trays 1, 2, 6 by manipulation of steam flow. The parameters tabulated to describe the column control performance of the column are the maximum deviation, offset, settling time and the I.S.E. values.

In all the graphs and tables in this section, the following units are used.

X_D	: weight per cent methanol
X_W	: weight per cent methanol
T_i	: °F
Maximum deviation (M.D.)	: weight per cent methanol
Offset (Off.)	: weight per cent methanol
Settling time (S.T.)	: minutes
τ_I	: minutes
K_c (for the temperature controller)	: $\frac{\text{lb./min.}}{°\text{F}}$
K_c (for the composition controller)	: $\frac{\text{lb./min.}}{\text{weight per cent methanol}}$
K_{FF}	: $\frac{\text{lb./min.}}{\text{weight per cent methanol}}$

X_D, X_W, T_i are the deviation variables.

A. Manipulation of reflux flow

(i) Feedback control of the liquid temperature on an intermediate tray.

Summary of results	- Table 6.4-15
Typical column responses	- Figures 6.4-26, 6.4-27 and 6.4-28

(ii) Feedforward plus feedback control of the liquid temperature on an intermediate tray using a proportional controller in the feedback loop.

Summary of results	- Table 6.4-16
Typical column responses	- Figures 6.4-29, 6.4-30 and 6.4-31

(iii) Feedforward plus feedback control of the liquid temperature on an intermediate tray using a PI controller in the feedback loop, τ_I = 10.0 minutes

Summary of results	- Table 6.4-17
Typical column responses	- Figures 6.4-32, 6.4-33 and 6.4-34

(iv) Feedforward plus feedback control of the liquid temperature on an intermediate tray using a PI controller in the feedback loop, τ_I = 1.0 minutes.

Summary of results	- Table 6.4-18
Typical column responses	- Figures 6.4-35, 6.4-36 and 6.4-37

(v) Feedback control and combined feedforward-feedback control of top product composition.

Summary of results - Table 6.4-19

(vi) Feedback control and combined feedforward-feedback control of bottom product composition.

Summary of results - Table 6.4-20

B. Manipulation of steam flow

(i) Feedback control of the liquid temperature on an intermediate tray.

Summary of results - Table 6.4-21

Typical column responses - Figures 6.4-38, 6.4-39 and 6.4-40

(ii) Feedforward plus feedback control of the liquid temperature on an intermediate tray using a proportional controller in the feedback loop.

Summary of results - Table 6.4-22

Typical column responses - Figures 6.4-41, 6.4-42 and 6.4-43

(iii) Feedforward plus feedback control of the liquid temperature on an intermediate tray using a PI controller in the feedback loop, τ_I = 10.0 minutes

Summary of results - Table 6.4-23

Typical column responses - Figures 6.4-44, 6.4-45 and 6.4-46

(iv) Feedforward plus feedback control of the liquid temperature on an intermediate tray using a PI controller in the feedback loop, τ_I = 1.0 minutes.

Summary of results	- Table 6.4-24
Typical column responses	- Figures 6.4-47, 6.4-48 and 6.4-49

(v) Feedback control and combined feedforward-feedback control of top product composition.

Summary of results	- Table 6.4-25

(vi) Feedback control and combined feedforward-feedback control of bottom product composition .

Summary of results	- Table 6.4-26

The case of feedforward plus feedback control of the liquid temperature on an intermediate tray using a PI feedback controller with τ_I = 100.0 minutes is not investigated here since the simulation results in section 6.4-1 and preliminary results revealed that with τ_I = 100.0 minutes, not enough intergral action is added and the results are nearly the same as the case of feedforward plus feedback control of the liquid temperature on an intermediate tray using a proportional feedback controller.

Table 6-4.15

Feedback Control of the Liquid Temperature on an Intermediate Tray

by Manipulation of Reflux Flow

(University of Alberta Column)

Control Tray		1	2	3	4	5	6	7	8
Optimum controller settings	K_c	-0.18	-0.15	-0.18	-0.30	-0.55	-1.00	-3.25	-224.0
	τ_I	15.0	26.0	20.0	13.0	10.0	5.0	2.0	1.2
X_D	M.D.	-3.61	-2.17	-2.04	-1.99	-1.44	-0.85	-0.59	-0.41
	Off.	-3.61	-2.17	-2.04	-1.99	-1.44	-0.85	-0.59	-0.41
	S.T.	85.	85.	85.	84.	83.	86.	94.	97.
	I.S.E.	1043.	438.9	404.8	354.4	183.6	61.55	25.22	12.36
X_W	M.D.	0.42	0.35	0.37	0.38	0.52	0.67	0.74	0.77
	Off.	-0.03	0.34	0.37	0.38	0.52	0.67	0.73	0.77
	S.T.	110.	82.	70.	63.	60.	58.	66.	63.
	I.S.E.	1.248	10.19	11.17	13.19	26.00	43.84	54.90	60.66
T_i	M.D.	-2.89	-3.93	-3.17	-1.52	-0.21	-0.17	-0.02	0.00
	Off.	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	S.T.	56.	102.	95.	34.	31.	15.	2.	0.
	I.S.E.	52.31	104.3	49.08	9.597	1.424	0.1278	0.0024	0.000

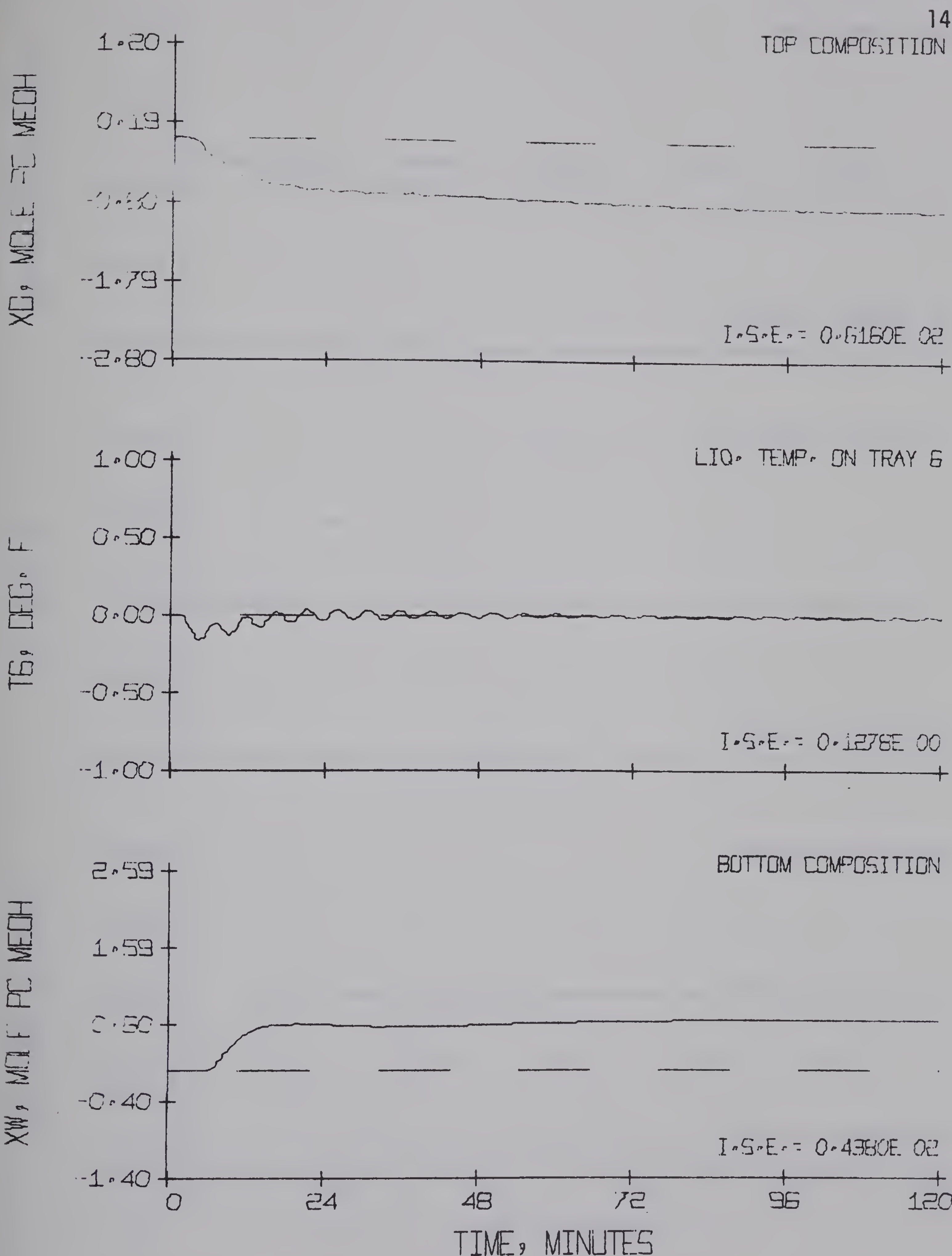
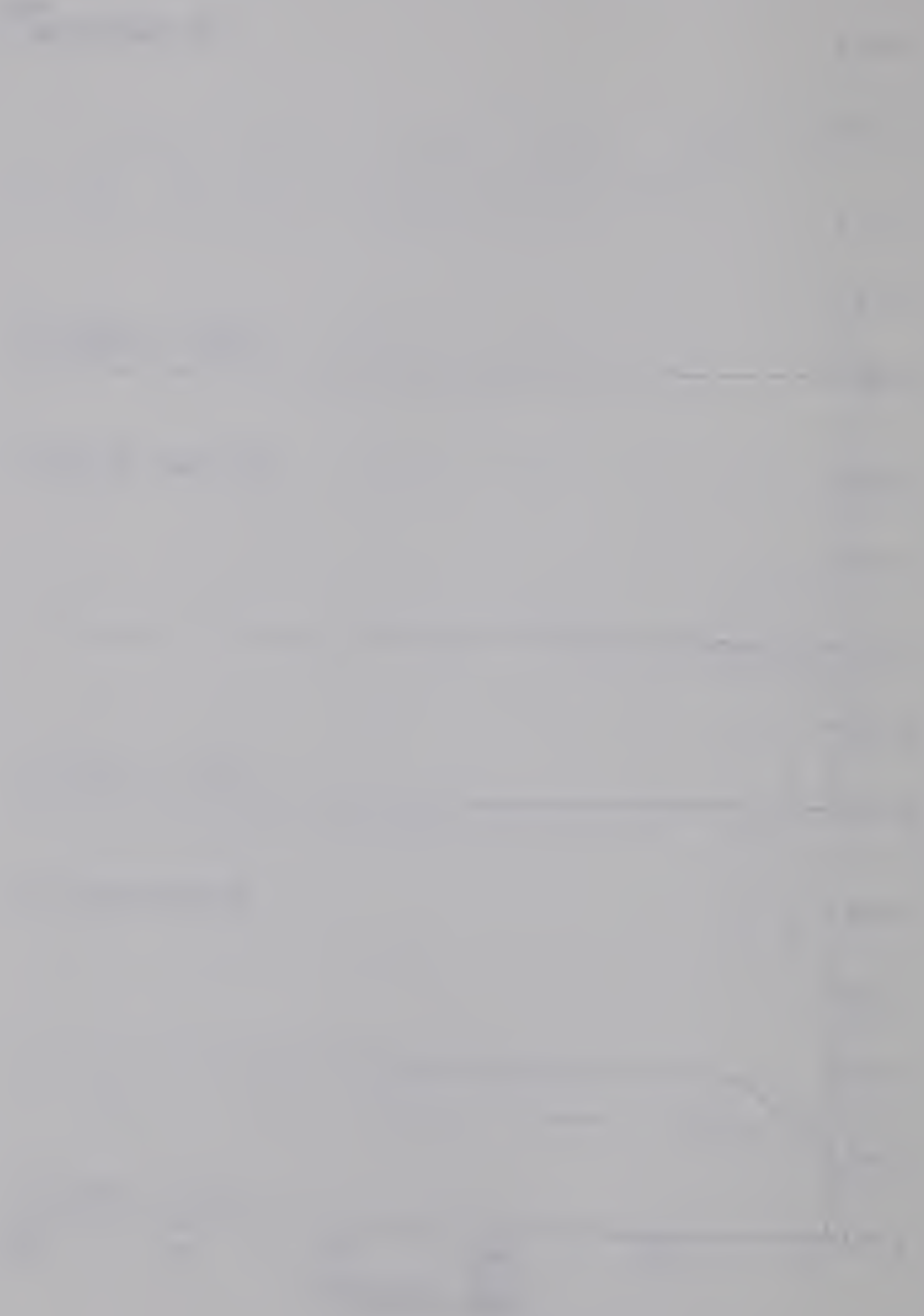


Figure 6.4-26 Feedback Control of the Liquid Temperature on Tray 6 by Manipulation of Reflux Flow (University of Alberta Column)



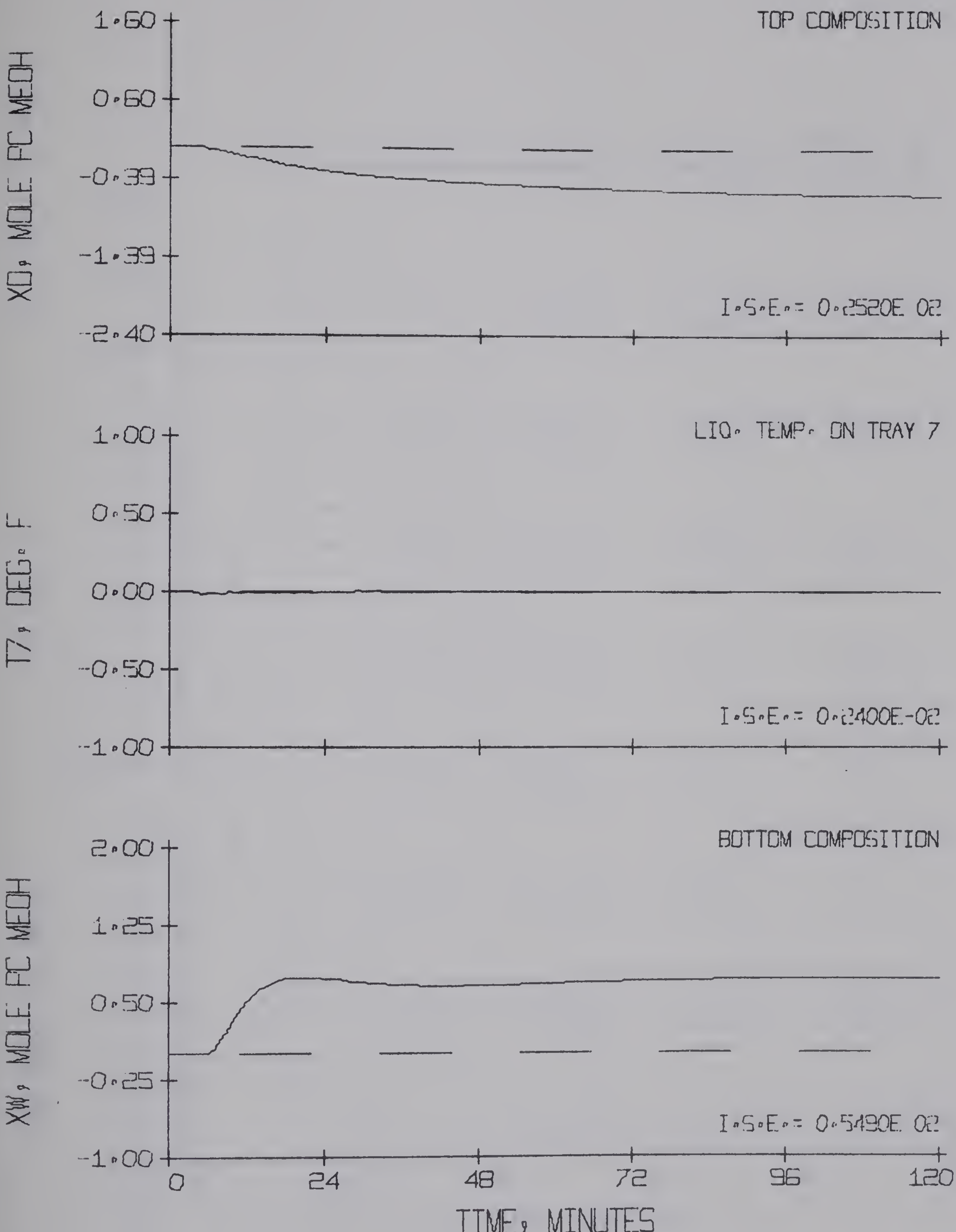


Figure 6.4-27 Feedback Control of the Liquid Temperature on Tray 7 by Manipulation of Reflux Flow (University of Alberta Column)

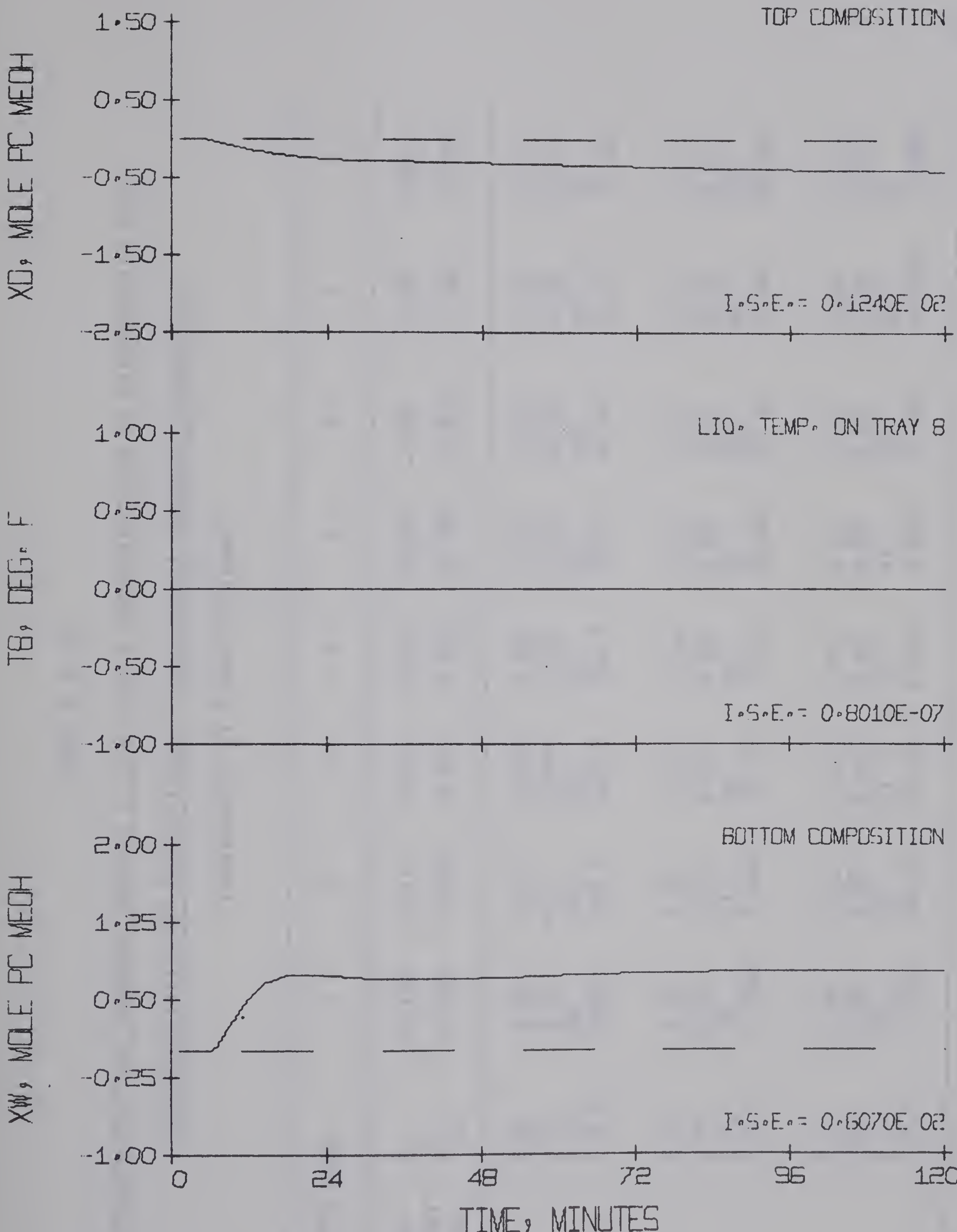


Figure 6.4-28 Feedback Control of the Liquid Temperature on Tray 8 by Manipulation of Reflux Flow (University of Alberta Column)

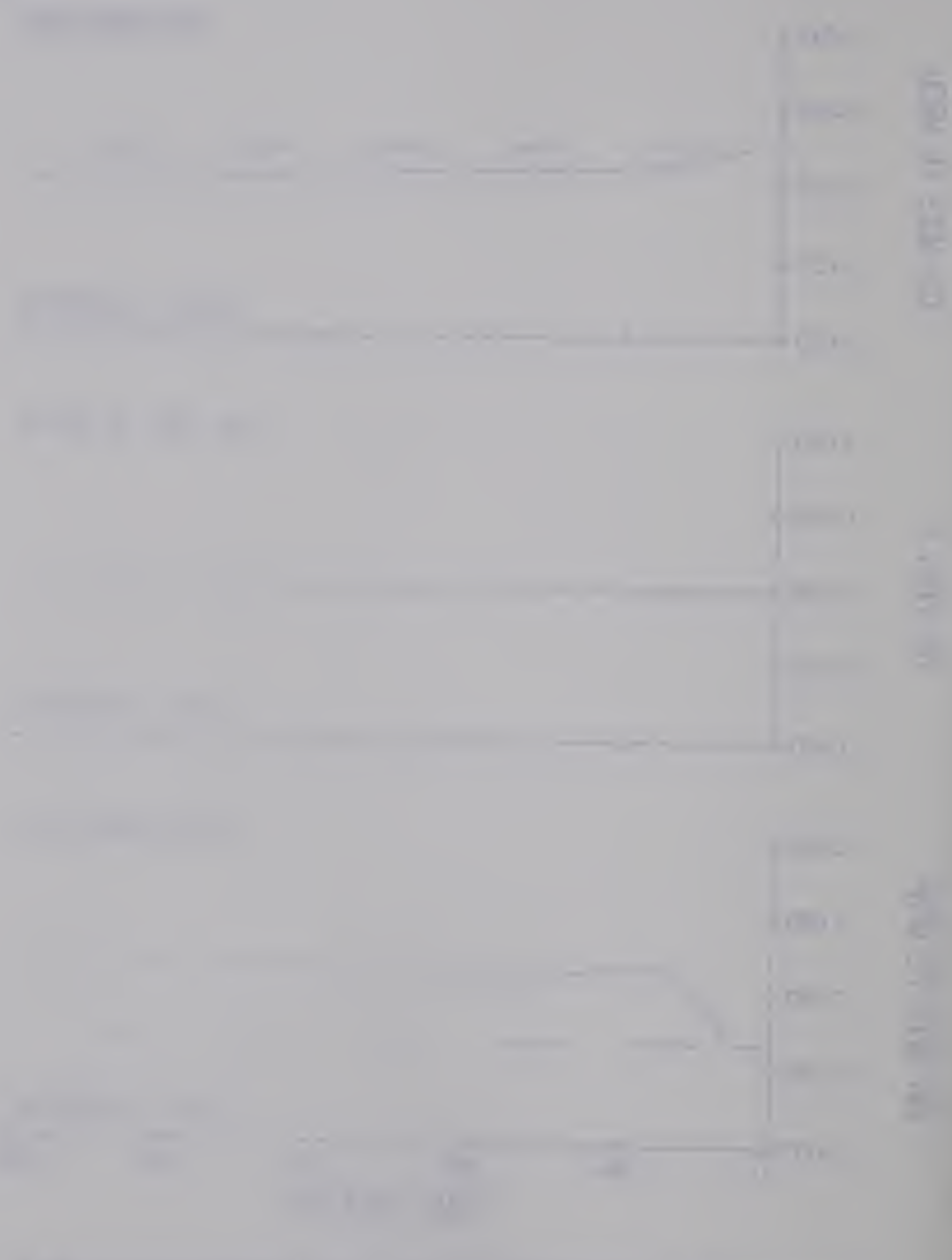


Table 6.4-16

Feedforward Plus Feedback Control of the Liquid Temperature on an Intermediate Tray by Manipulation of Reflux Flow - Proportional Feedback Controller

(University of Alberta Column)

Control Tray		1	2	3	4	5	6	7	8
Optimum controller settings	K_c	-0.135	-0.12	-0.15	-0.25	-0.50	-1.00	-3.45	-220.0
	K_{FF}	-0.762	-0.587	-0.571	-0.566	-0.500	-0.430	-0.361	-0.378
X_D	M.D.	-3.62	-2.17	-2.04	-1.99	-1.44	-0.85	-0.59	-0.41
	Off.	-3.62	-2.17	-2.04	-1.99	-1.44	-0.85	-0.59	-0.41
	S.T.	78.	75.	73.	72.	80.	87.	94.	97.
	I.S.E.	1095.	451.5	401.9	354.9	181.2	61.45	25.14	12.36
X_W	M.D.	0.21	0.34	0.37	0.38	0.52	0.67	0.75	0.77
	Off.	-0.03	0.34	0.37	0.38	0.52	0.67	0.75	0.77
	S.T.	76.	71.	68.	62.	67.	66.	65.	63.
	I.S.E.	0.2984	8.895	10.73	12.61	25.36	43.81	54.90	60.66
T_i	M.D.	-1.24	-2.53	-2.00	-0.89	0.27	0.27	0.08	0.00
	Off.	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	S.T.	37.	35.	31.	12.	41.	34.	33.	0.
	I.S.E.	7.280	28.63	15.82	2.562	0.0327	0.1641	0.0140	0.0000

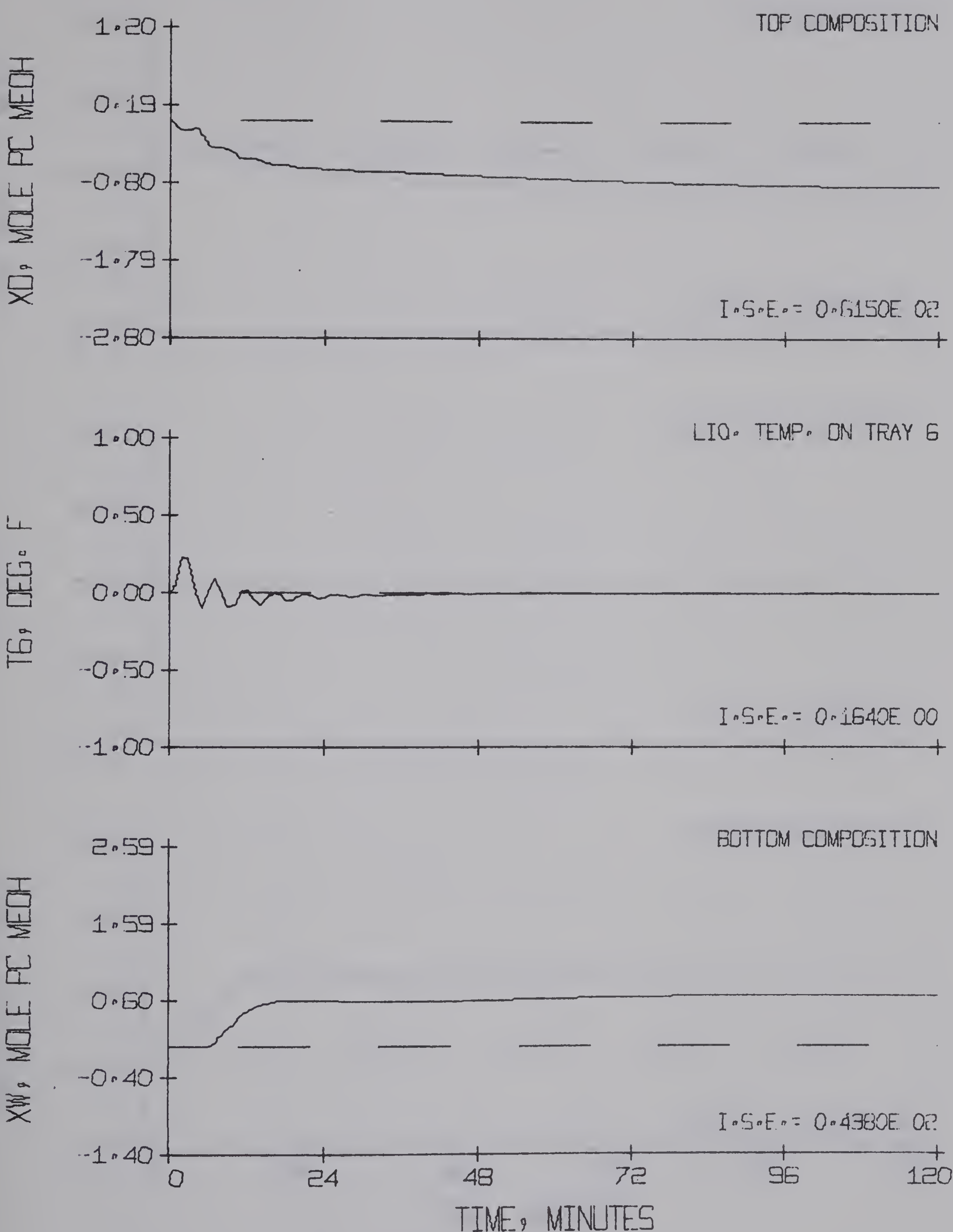


Figure 6.4-29 Feedforward Plus Feedback Control of the Liquid Temperature on Tray 6 by Manipulation of Reflux Flow - Proportional Controller Only (University of Alberta Column)

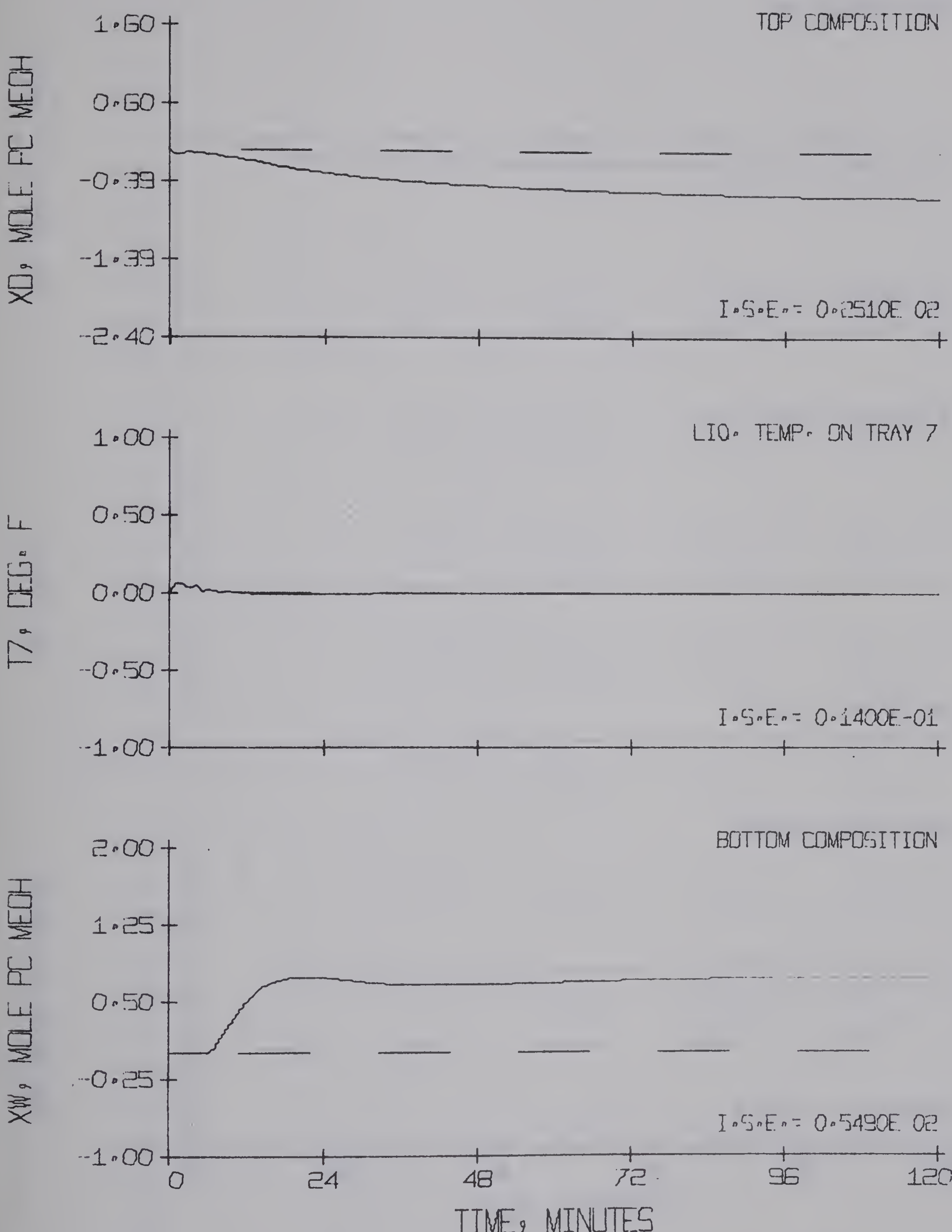


Figure 6.4-30 Feedforward Plus Feedback Control of the Liquid Temperature on Tray 7 by Manipulation of Reflux Flow - Proportional Feedback Controller (University of Alberta Column)

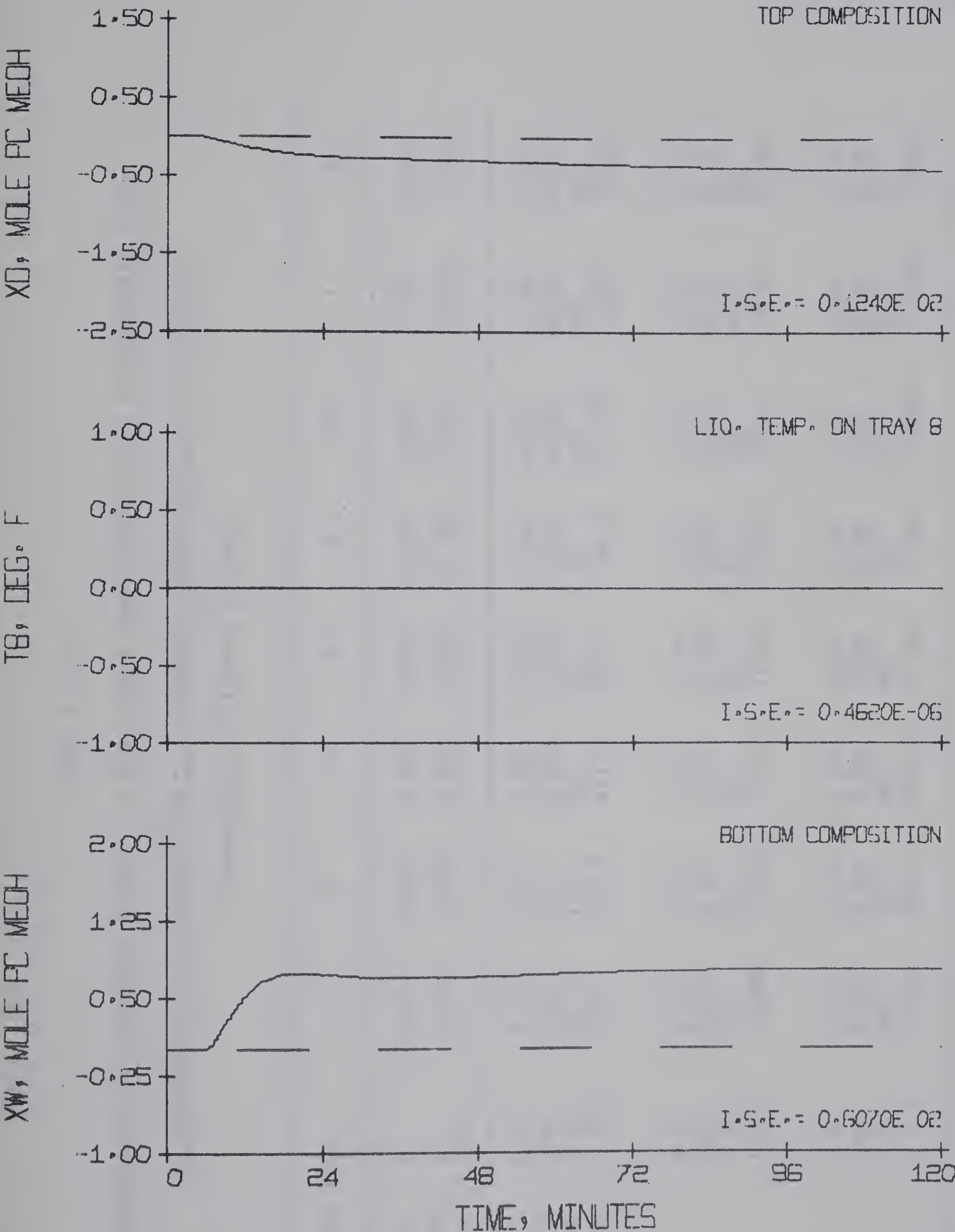


Figure 6.4-31 Feedforward Plus Feedback Control of the Liquid Temperature on Tray 8 by Manipulation of Reflux Flow - Proportional Feedback Controller (University of Alberta Column)

Table 6.4-17

Feedforward Plus Feedback Control of the Liquid Temperature on an Intermediate Tray by Manipulation of Reflux Flow - PI Feedback Controller, τ_I = 10.0 min.

(University of Alberta Column)

Control Tray		1	2	3	4	5	6	7	8
Optimum controller settings	K_I	-0.10	-0.08	-0.115	-0.215	-0.45	-0.95	-3.25	-200.0
	K_{FF}	-0.762	-0.587	-0.571	-0.566	-0.500	-0.430	-0.361	-0.378
X_D	M.D.	-3.62	-2.17	-2.04	-1.99	-1.44	-0.85	-0.59	-0.41
	Off.	-3.62	-2.17	-2.04	-1.99	-1.44	-0.85	-0.59	-0.41
	S.T.	79.	77.	76.	74.	81.	87.	94.	97.
	I.S.E.	1111.	478.2	411.8	361.0	180.9	61.79	25.22	12.36
X_W	M.D.	0.21	0.34	0.37	0.38	0.52	0.67	0.75	0.77
	Off.	-0.03	0.34	0.37	0.38	0.52	0.67	0.75	0.77
	S.T.	78.	72.	70.	66.	66.	66.	65.	63.
	I.S.E.	0.3458	9.000	10.49	12.38	25.00	43.76	54.91	60.66
T_i	M.D.	-1.25	-2.74	-2.09	-0.92	0.32	0.28	0.09	0.00
	Off.	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	S.T.	38.	38.	42.	44.	37.	37.	26.	0.
	I.S.E.	11.26	44.67	22.27	3.349	0.4001	0.2075	0.0130	0.0000

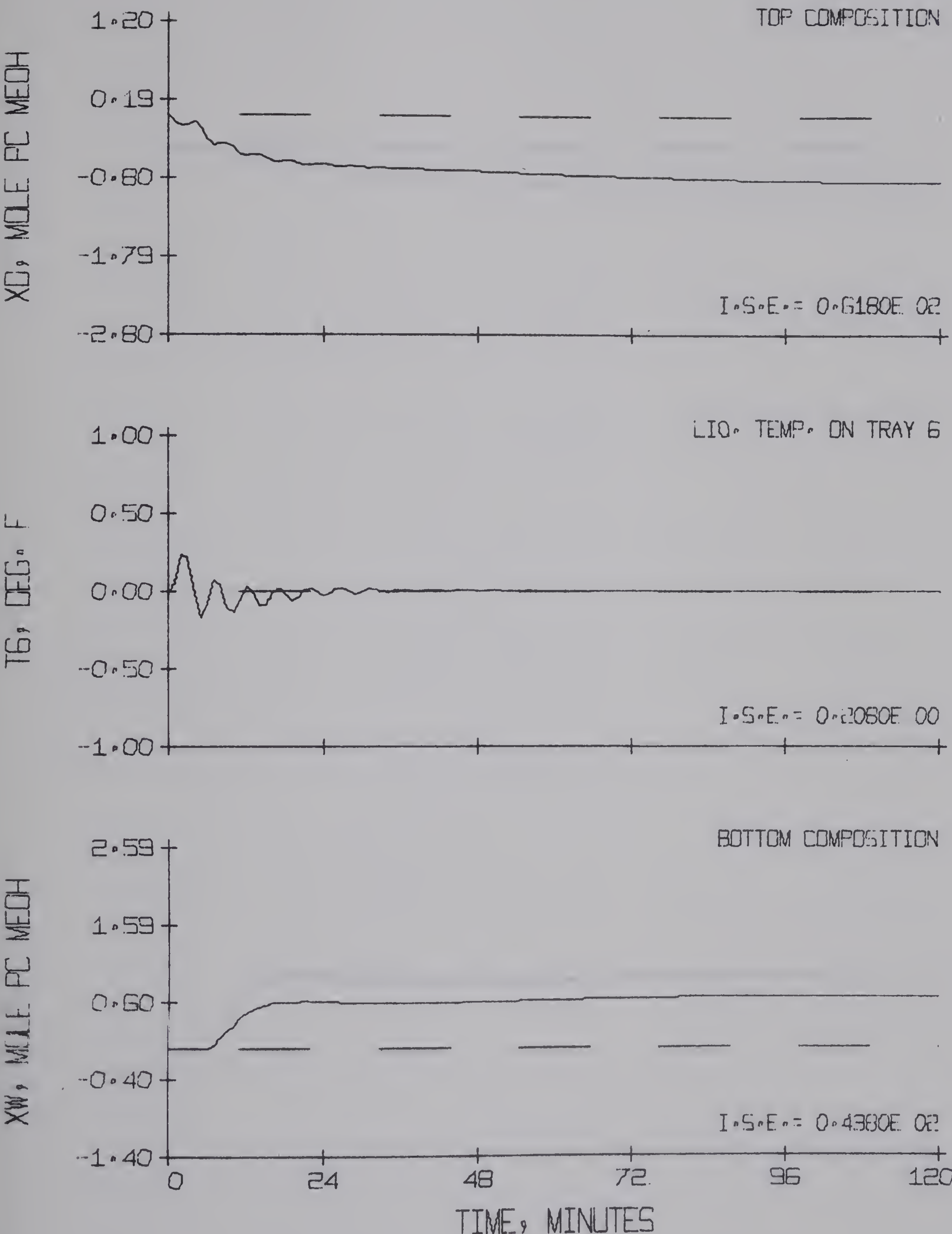


Figure 6.4-32 Feedforward Plus Feedback Control of the Liquid Temperature on Tray 6 by Manipulation of Reflux Flow - PI Feedback Controller, τ_I = 10.0 min. (University of Alberta Column)

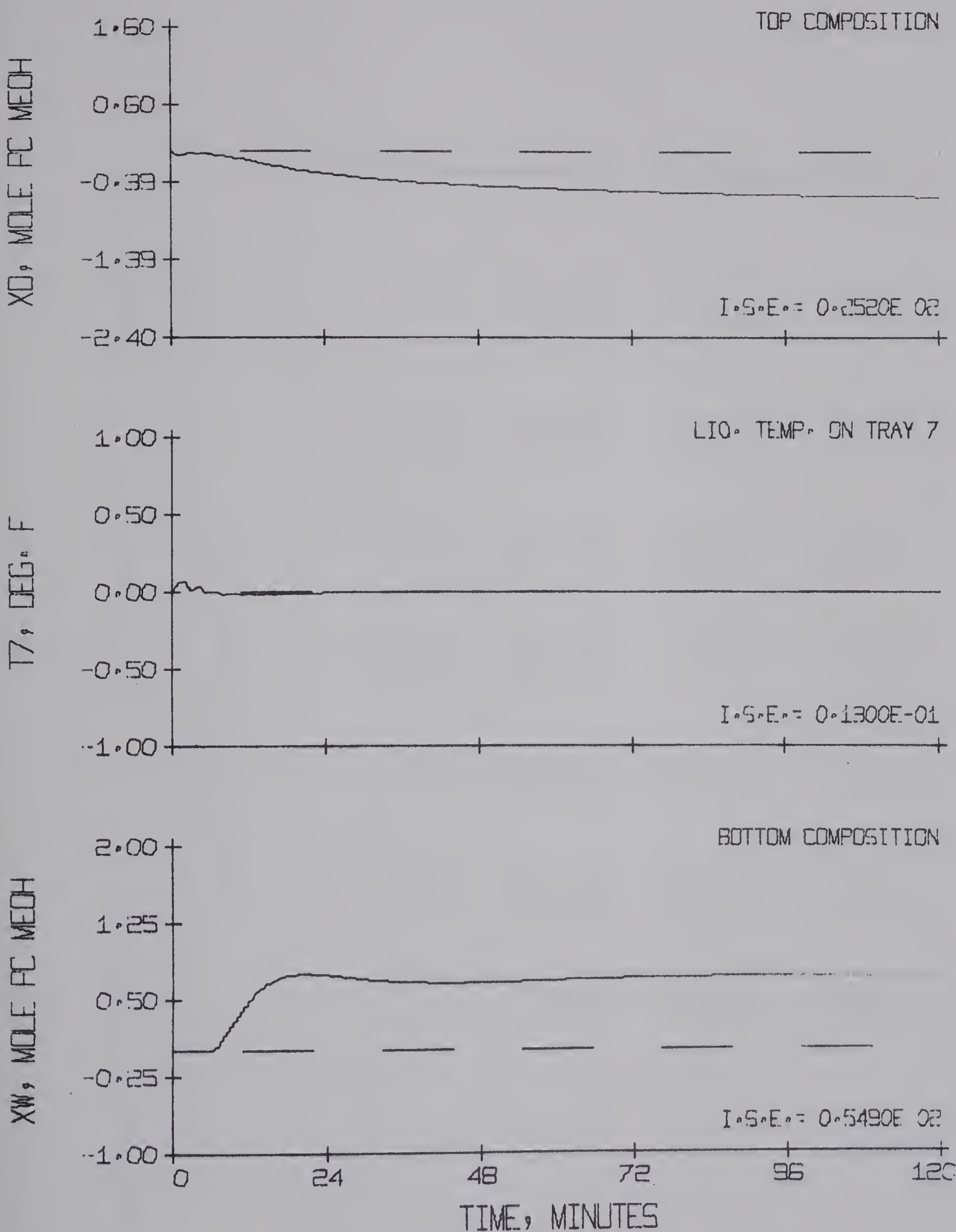


Figure 6.4-33 Feedforward Plus Feedback Control of the Liquid Temperature on Tray 7 by Manipulation of Reflux Flow - PI Feedback Controller, τ_I = 10.0 min. (University of Alberta Column)

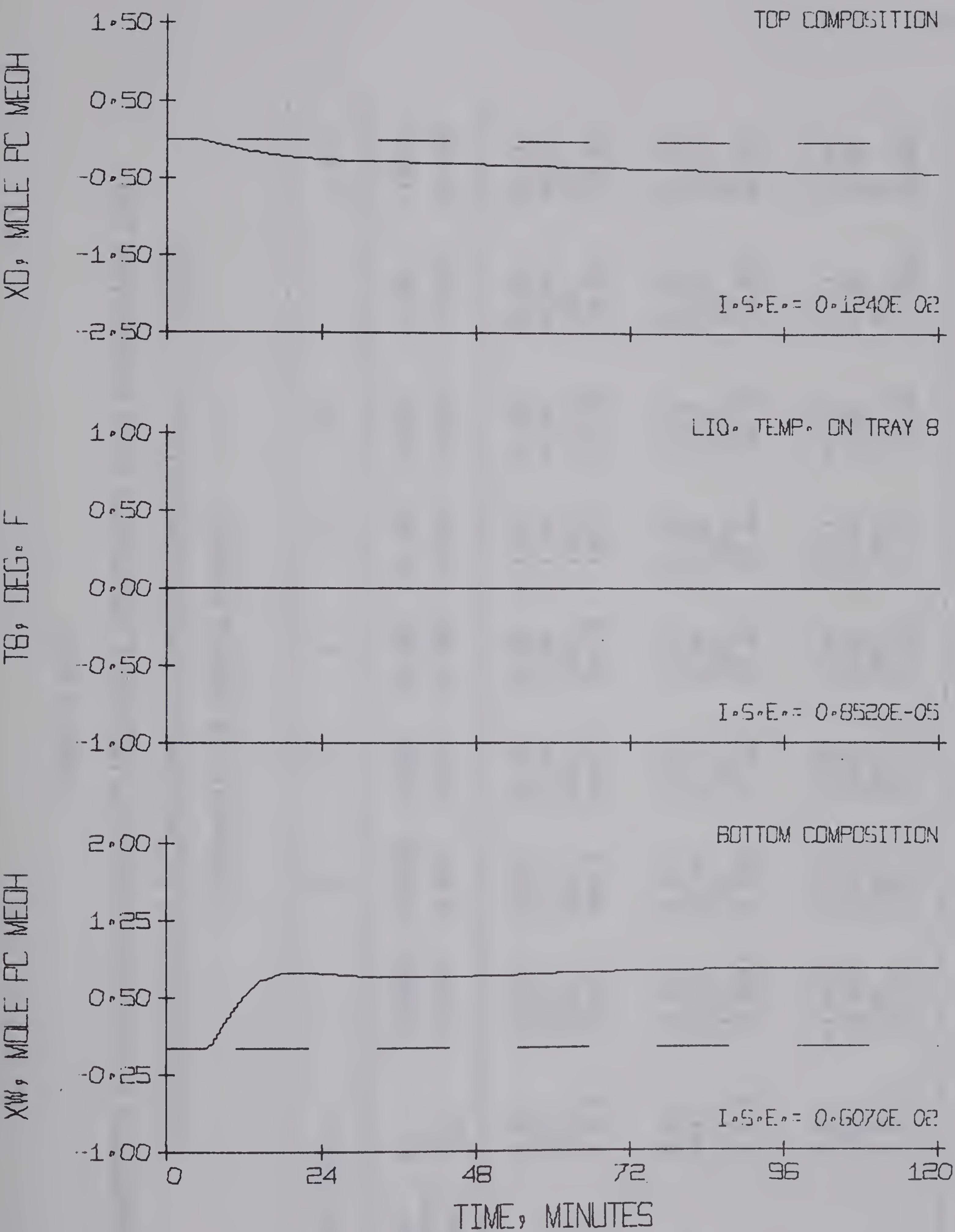


Figure 6.4-34 Feedforward Plus Feedback Control of the Liquid Temperature on Tray 8 by Manipulation of Reflux Flow - PI Feedback Controller, τ_I = 10.0 min. (University of Alberta Column)

Table 6.4-18

Feedforward Plus Feedback Control of the Liquid Temperature on an Intermediate Tray by Manipulation of Reflux Flow - PI Feedback Controller, τ_I = 1.0 min.

(University of Alberta Column)

Control Tray		1	2	3	4	5	6	7	8
Otpimum controller settings	K_c	-0.0004	-0.0008	-0.002	-0.004	-0.007	-0.04	-1.60	-150.0
	K_{FF}	-0.762	-0.587	-0.571	-0.566	-0.500	-0.430	-0.361	-0.378
X_D	M.D.	-3.70	-2.66	-2.28	-2.06	-1.51	-0.95	-0.59	-0.41
	Off.	-3.70	-2.17	-2.04	-1.99	-1.44	-0.90	-0.59	-0.41
	S.T.	120.	120.	120.	120.	120.	117.	94.	97.
	I.S.E.	1103.	489.5	429.5	374.9	184.5	63.49	25.27	12.37
X_W	M.D.	0.24	0.57	0.45	0.43	0.55	0.73	0.75	0.77
	Off.	-0.03	0.34	0.37	0.38	0.52	0.67	0.73	0.77
	S.T.	120.	120.	120.	120.	120.	108.	65.	63.
	I.S.E.	0.9535	8.084	11.46	12.66	25.44	44.38	54.89	60.67
T_i	M.D.	-1.40	-3.70	-2.80	-1.24	-0.71	-0.81	0.11	0.00
	Off.	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	S.T.	120.	120.	120.	120.	120.	120.	65.	0.
	I.S.E.	25.00	282.8	205.1	32.98	12.94	13.58	0.0530	0.0000

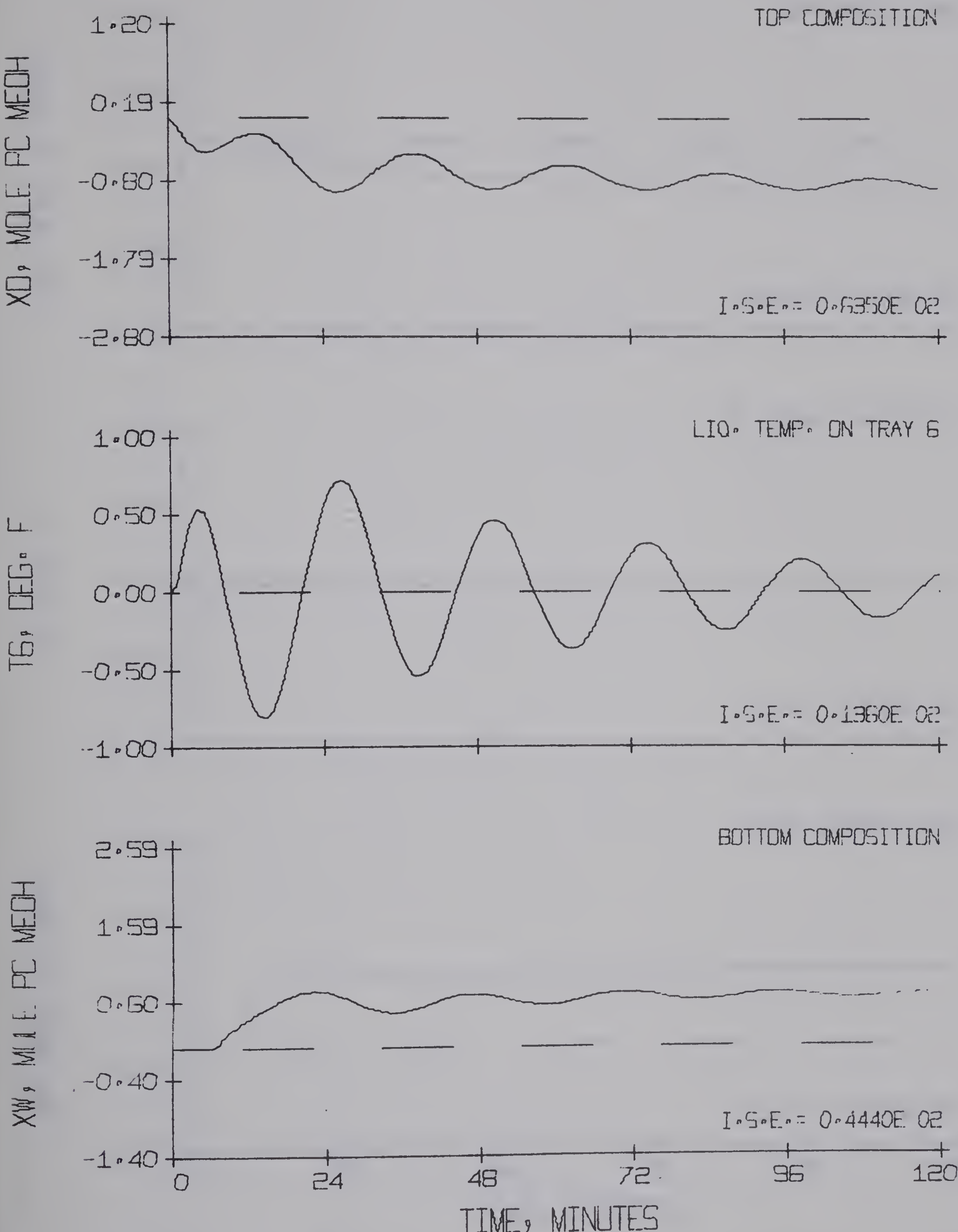


Figure 6.4-35 Feedforward Plus Feedback Control of the Liquid Temperature on Tray 6 by Manipulation of Reflux Flow - PI Feedback Controller, τ_I = 1.0 min. (University of Alberta Column)

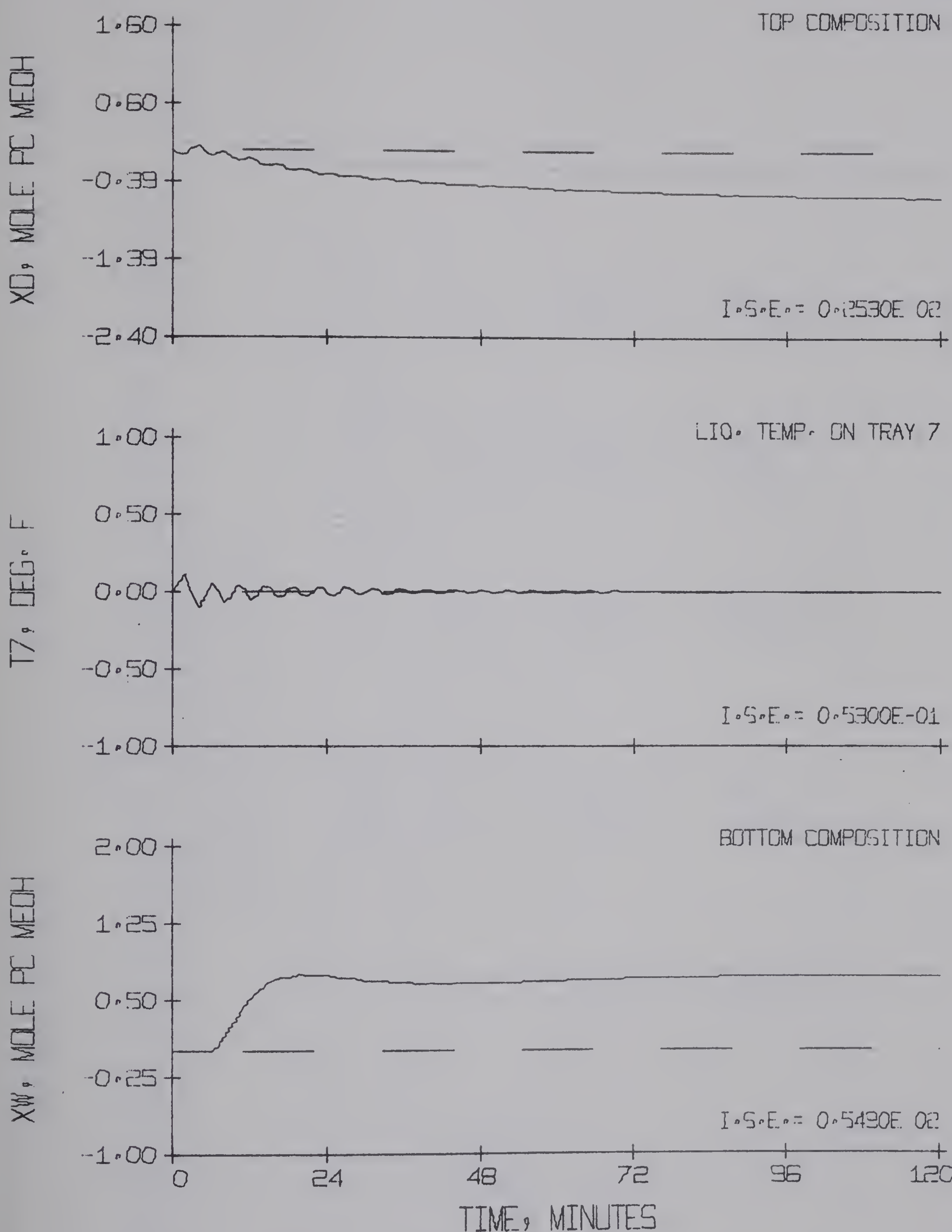


Figure 6.4-36 Feedforward Plus Feedback Control of the Liquid Temperature on Tray 7 by Manipulation of Reflux Flow - PI Feedback Controller, τ_I = 1.0 min. (University of Alberta Column)

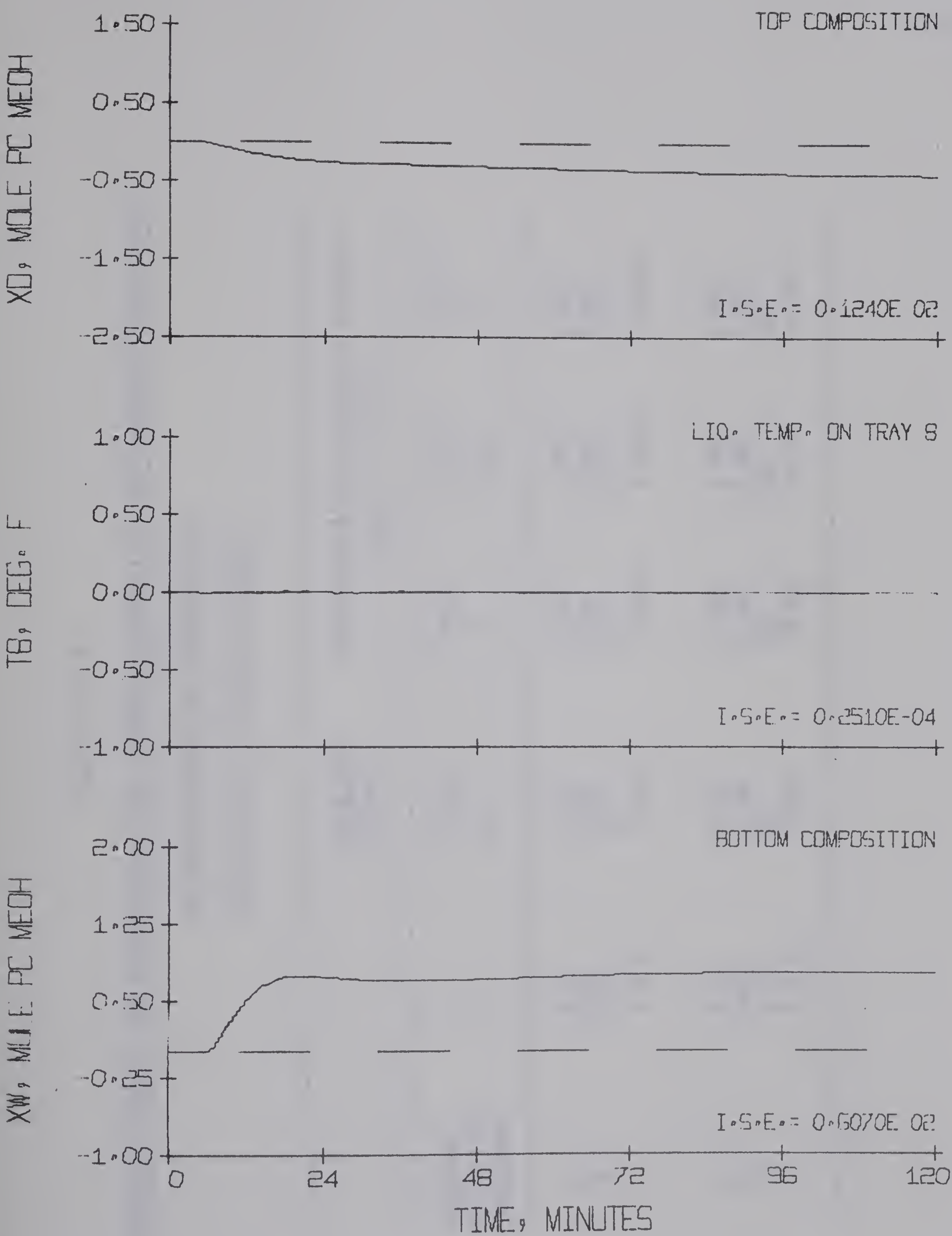


Figure 6.4-37 Feedforward Plus Feedback Control of the Liquid Temperature on Tray 8 by Manipulation of Reflux Flow - PI Feedback Controller, τ_I = 1.0 min. (University of Alberta Column)

Table 6.4-19

Feedback Control and Feedforward Plus Feedback Control of Top Product Composition

by Manipulation of Reflux Flow

(University of Alberta Column)

		Feedback Control	Feedforward Plus Feedback Control $K_{FF} = -0.327$		
Optimum controller constants	K_c	725.0	700.0	600.0	120.0
	τ_I	3.0	∞	10.0	1.0
X_D	M.D.	0.00	0.00	0.00	0.00
	Off.	0.00	0.00	0.00	0.00
	S.T.	2.	2.	2.	4.
	I.S.E.	0.0000	0.0000	0.0000	0.0000
X_W	M.D.	0.88	0.88	0.88	0.88
	Off.	0.88	0.88	0.88	0.88
	S.T.	62.	62.	62.	65.
	I.S.E.	75.98	75.98	75.98	75.99

Table 6.4-20

Feedback Control and Feedforward Plus Feedback Control of Bottom Product Composition

by Manipulation of Reflux Flow

(University of Alberta Column)

		Feedback Control	Feedforward plus Feedback Control $K_{FF} = -0.747$		
Optimum controller constants	K_c	0.45	0.25	0.045	0.00065
	τ_I	26.0	∞	10.0	1.0
X_D	M.D.	-3.55	-3.55	-3.55	-3.55
	Off.	-3.55	-3.55	-3.55	-3.55
	S.T.	104.	98.	98.	99.
	I.S.E.	798.3	1088.	1088.	988.5
X_W	M.D.	0.55	0.25	0.25	0.25
	Off.	0.00	0.00	0.00	0.00
	S.T.	85.	80.	80.	80.
	I.S.E.	10.77	0.6266	0.7276	0.8927

Table 6.4-21

Feedback Control of the Liquid Temperature on an Intermediate Tray

by Manipulation of Steam Flow

(University of Alberta Column)

Control Tray		1	2	3	4	5	6	7	8
Optimum controller settings	K_c	8.0	3.5	6.0	7.0	7.0	16.0	25.0	28.0
	τ_I	5.0	1.25	1.25	1.0	3.0	5.0	2.0	1.75
X_D	M.D.	-0.63	-0.67	-0.75	-0.69	-0.39	-0.20	0.51	0.39
	Off.	-0.08	-0.24	-0.39	-0.34	-0.07	0.02	0.51	0.39
	S.T.	102.	99.	91.	90.	110.	114.	87.	85.
	I.S.E.	12.42	19.71	32.52	25.96	5.578	1.208	17.13	8.674
X_W	M.D.	0.14	-0.14	-0.22	-0.19	0.17	0.34	0.50	0.38
	Off.	-0.04	-0.13	-0.22	-0.19	-0.04	0.02	0.29	0.23
	S.T.	93.	61.	42.	41.	86.	56.	58.	52.
	I.S.E.	0.4280	1.742	4.411	3.174	0.4512	1.698	12.22	7.444
T_i	M.D.	-0.09	0.09	0.01	0.00	0.01	-0.02	0.00	0.00
	Off.	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	S.T.	6.	5.	5.	1.	2.	6.	0.	0.
	I.S.E.	0.0054	0.0081	0.0030	0.0002	0.006	0.0040	0.0000	0.0000

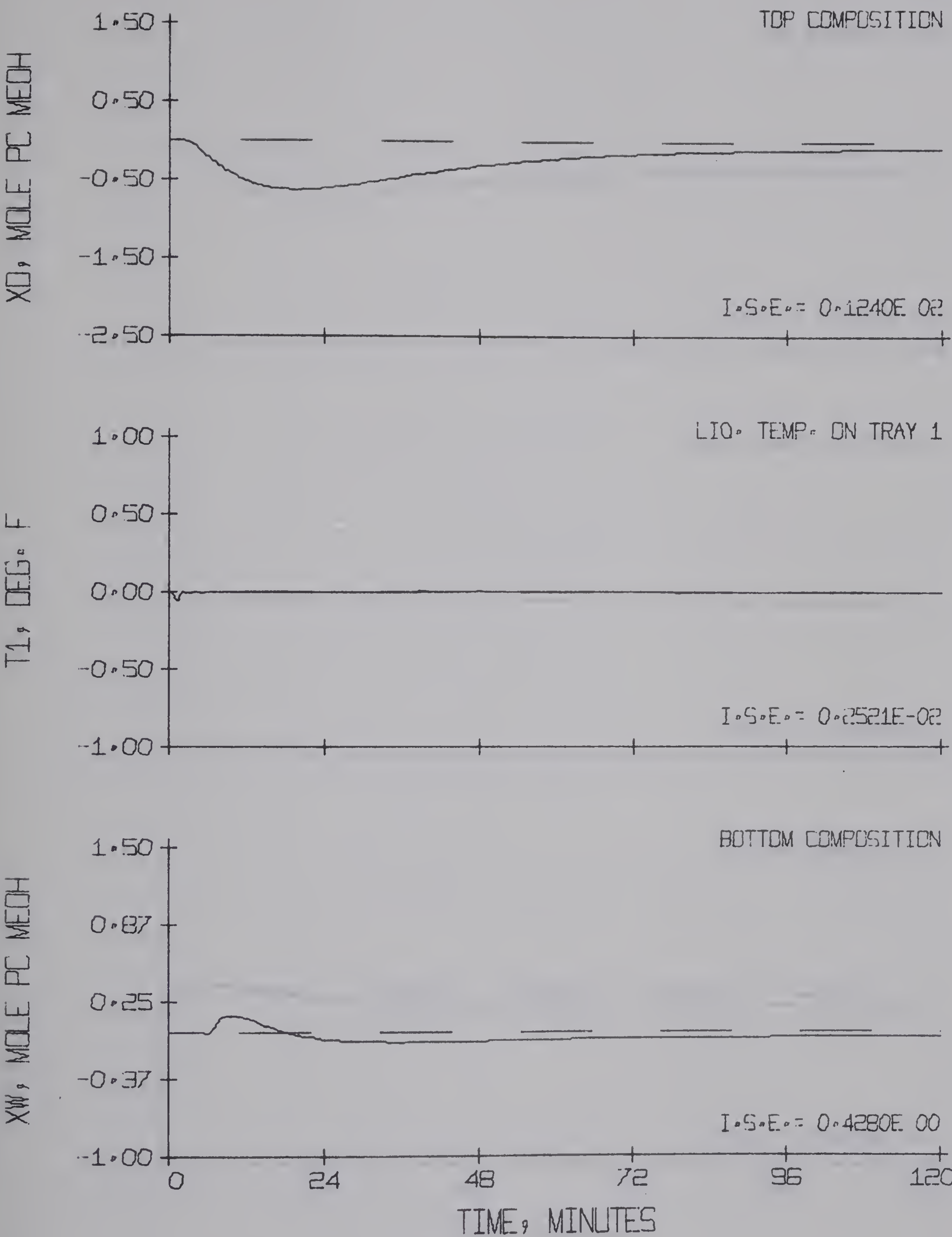


Figure 6.4-38 Feedback Control of the Liquid Temperature on Tray 1
by Manipulation of Steam Flow
(University of Alberta Column)

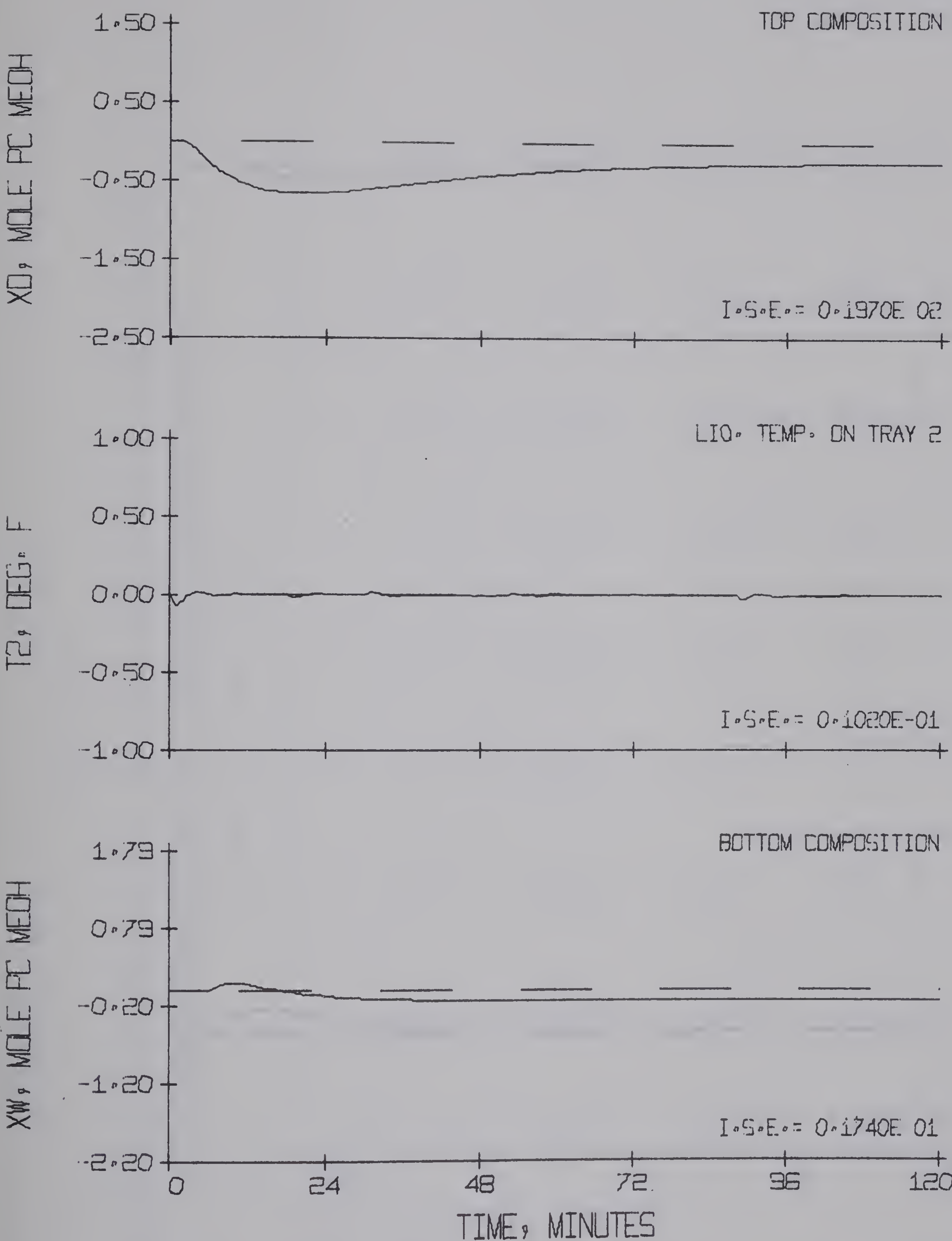


Figure 6.4-39 Feedback Control of the Liquid Temperature on Tray 2 by Manipulation of Steam Flow (University of Alberta Column)

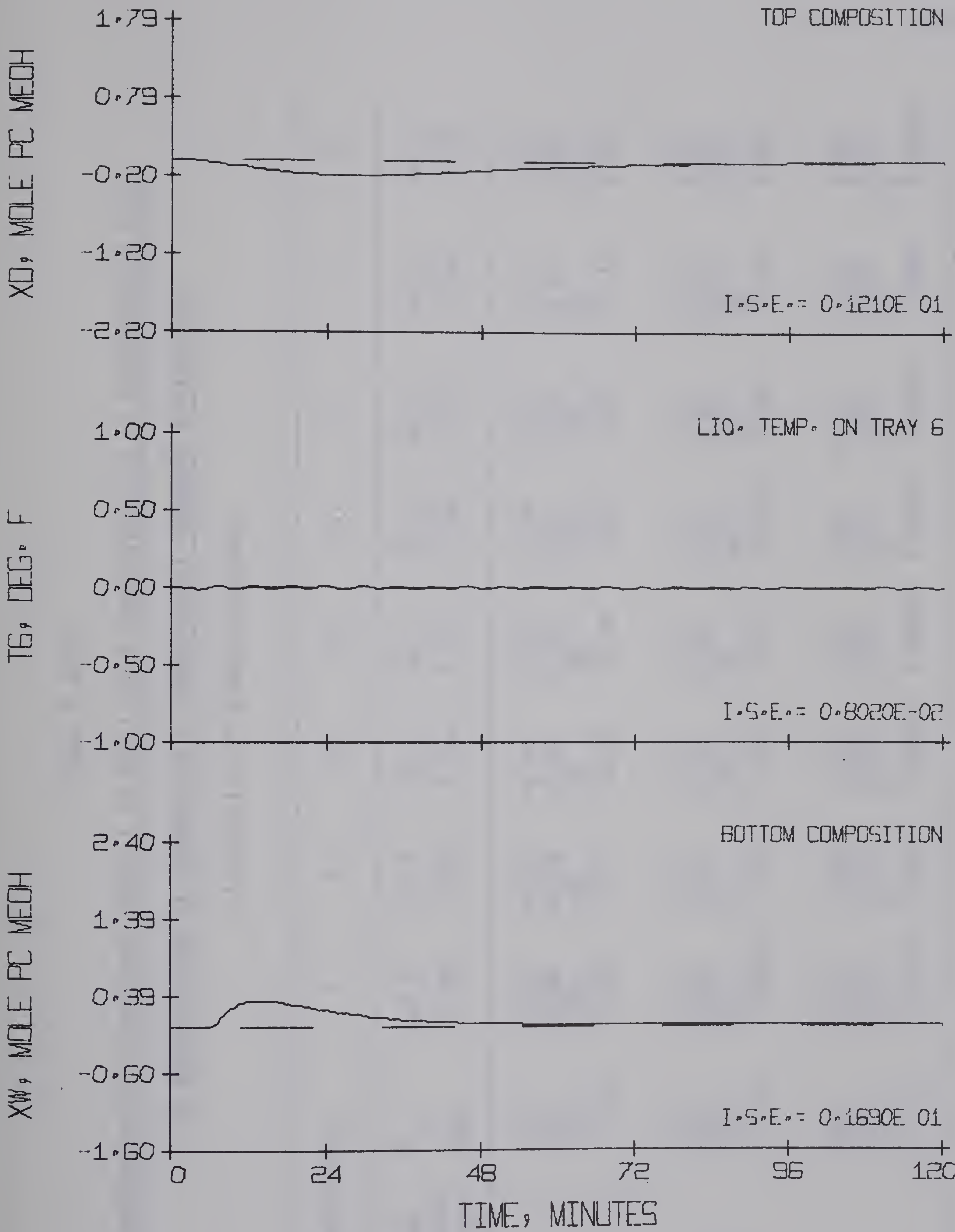


Figure 6.4-40 Feedback Control of the Liquid Temperature on Tray 6 by Manipulation of Steam Flow (University of Alberta Column)

Table 6.4-22

Feedforward Plus Feedback Control of the Liquid Temperature on an Intermediate Tray by Manipulation of Steam Flow - Proportional Feedback Controller

(University of Alberta Column)

Control Tray		1	2	3	4	5	6	7	8
Optimum controller settings	K_c	46.0	42.0	43.0	46.0	47.0	45.0	42.0	46.0
	K_{FF}	0.267	0.282	0.296	0.291	0.266	0.258	0.206	0.201
X_D	M.D.	-0.63	-0.67	-0.75	-0.69	0.39	-0.20	0.51	0.39
	Off.	-0.08	-0.24	-0.39	-0.34	-0.07	0.02	0.51	0.39
	S.T.	102.	99.	91.	90.	110.	114.	87.	85.
	I.S.E.	12.42	19.71	32.56	25.95	5.578	1.209	17.13	8.673
X_W	M.D.	0.14	-0.14	-0.22	-0.19	0.17	0.34	0.51	0.38
	Off.	-0.04	-0.13	-0.22	-0.19	-0.04	0.02	0.29	0.23
	S.T.	93.	61.	42.	41.	86.	56.	58.	45.
	I.S.E.	0.4280	1.742	4.412	3.174	0.4510	1.689	12.22	7.445
T_i	M.D.	-0.04	0.04	0.00	0.00	0.01	-0.02	0.00	0.00
	Off.	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	S.T.	6.	5.	2.	1.	2.	6.	0.	0.
	I.S.E.	0.0018	0.0025	0.0000	0.0000	0.0003	0.0040	0.0000	0.0000

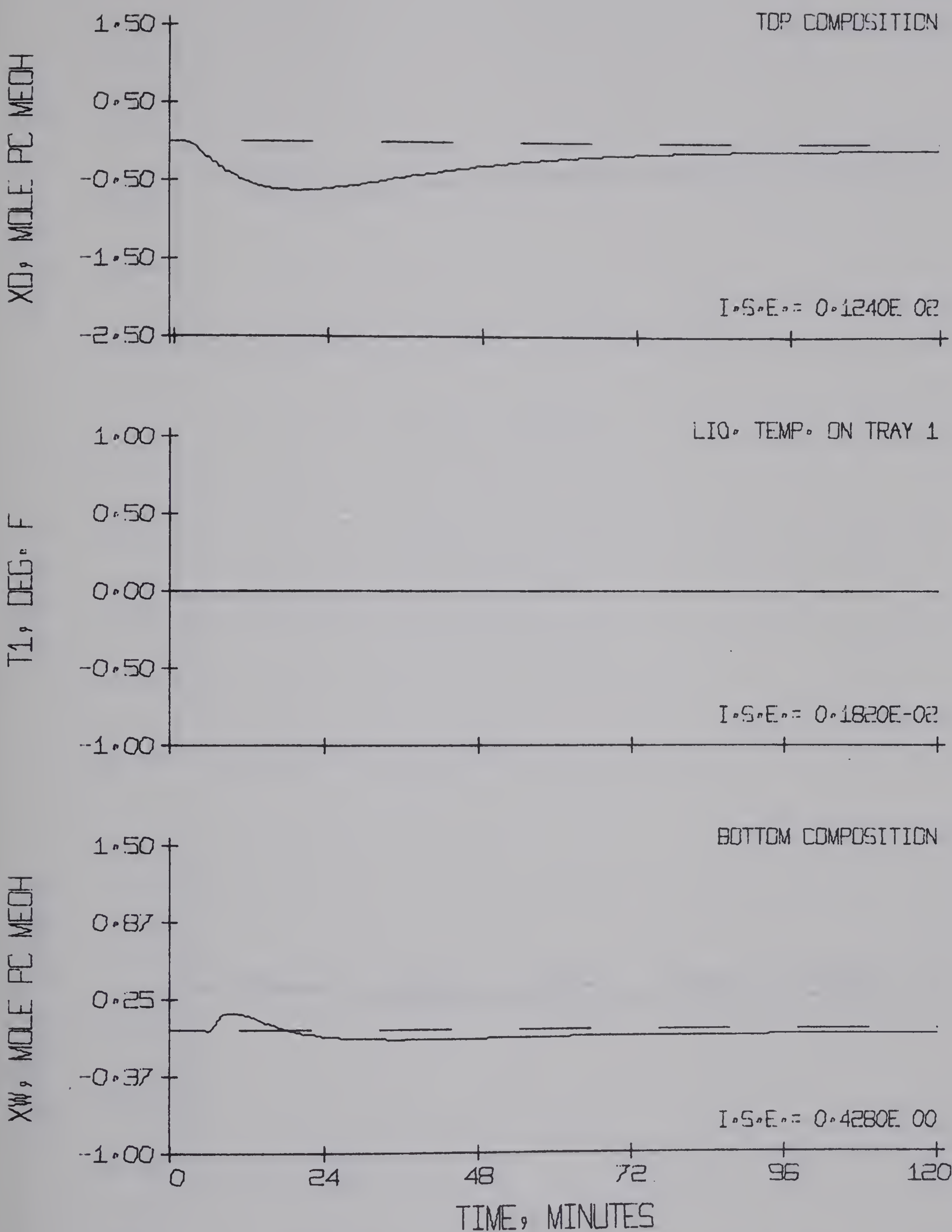


Figure 6.4-41 Feedforward Plus Feedback Control of the Liquid Temperature on Tray 1 by Manipulation of Steam Flow - Proportional Feedback Controller (University of Alberta Column)

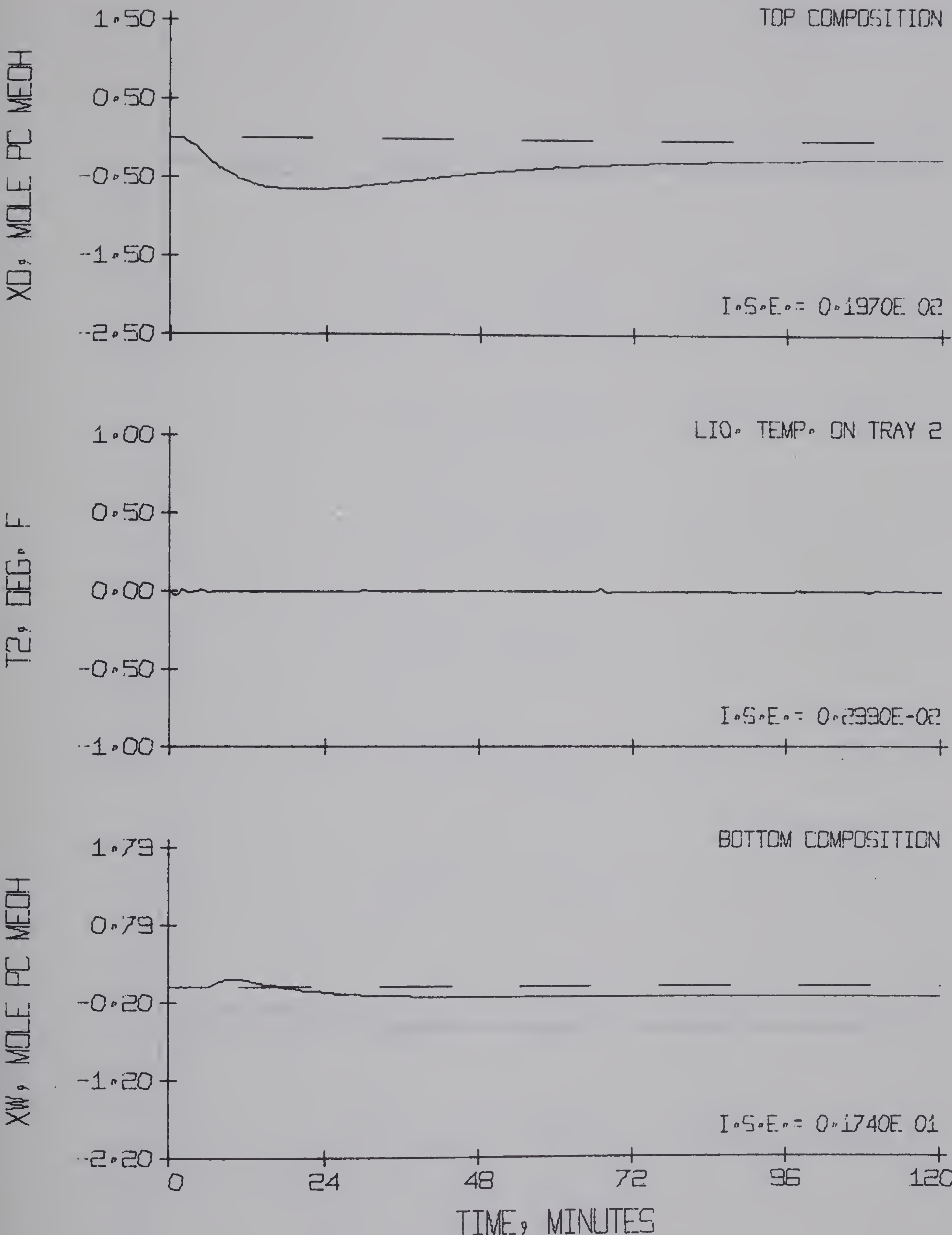


Figure 6.4-42 Feedforward Plus Feedback Control of the Liquid Temperature on Tray 2 by Manipulation of Steam Flow - Proportional Feedback Controller (University of Alberta Column)

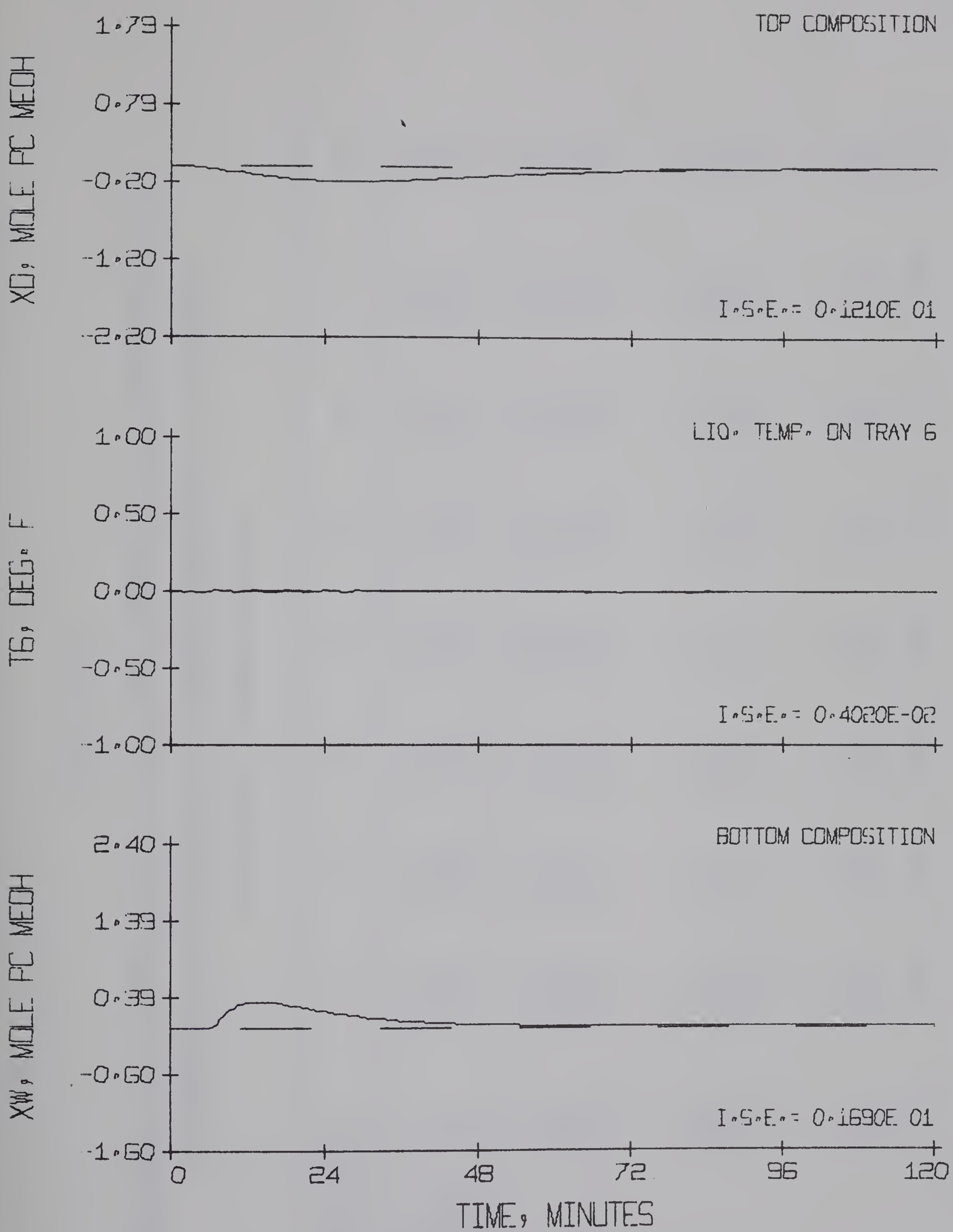


Figure 6.4-43 Feedforward Plus Feedback Control of the Liquid Temperature on Tray 6 by Manipulation of Steam Flow - Proportional Feedback Controller (University of Alberta Column)

Table 6.4-23

Feedforward Plus Feedback Control of the Liquid Temperature on an Intermediate Tray by Manipulation of Steam Flow - PI Feedback Controller, τ_I = 10.0 min.

(University of Alberta Column)

Control Tray		1	2	3	4	5	6	7	8
Optimum controller settings	K_c	32.0	35.0	35.0	34.0	31.0	31.0	32.0	31.0
	K_{FF}	0.267	0.282	0.296	0.291	0.266	0.258	0.206	0.201
X_D	M.D.	-0.63	-0.67	-0.75	-0.69	-0.39	-0.20	0.51	0.39
	Off.	-0.08	-0.24	-0.39	-0.34	-0.07	0.02	0.51	0.39
	S.T.	102.	99.	91.	90.	112.	111.	87.	85.
	I.S.E.	12.41	19.70	32.56	25.94	5.578	1.209	17.13	8.673
X_W	M.D.	0.14	-0.14	-0.22	-0.19	0.17	0.34	0.51	0.38
	Off.	-0.04	-0.13	-0.22	-0.19	-0.04	0.02	0.29	0.23
	S.T.	93.	61.	42.	41.	86.	56.	58.	45.
	I.S.E.	0.4280	1.741	4.412	3.175	0.4512	1.687	12.21	7.446
T_i	M.D.	-0.05	0.06	0.01	0.02	0.01	-0.02	0.00	0.00
	Off.	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	S.T.	6.	5.	3.	2.	2.	4.	0.	0.
	I.S.E.	0.0021	0.0031	0.0008	0.0012	0.0008	0.0041	0.0001	0.0002

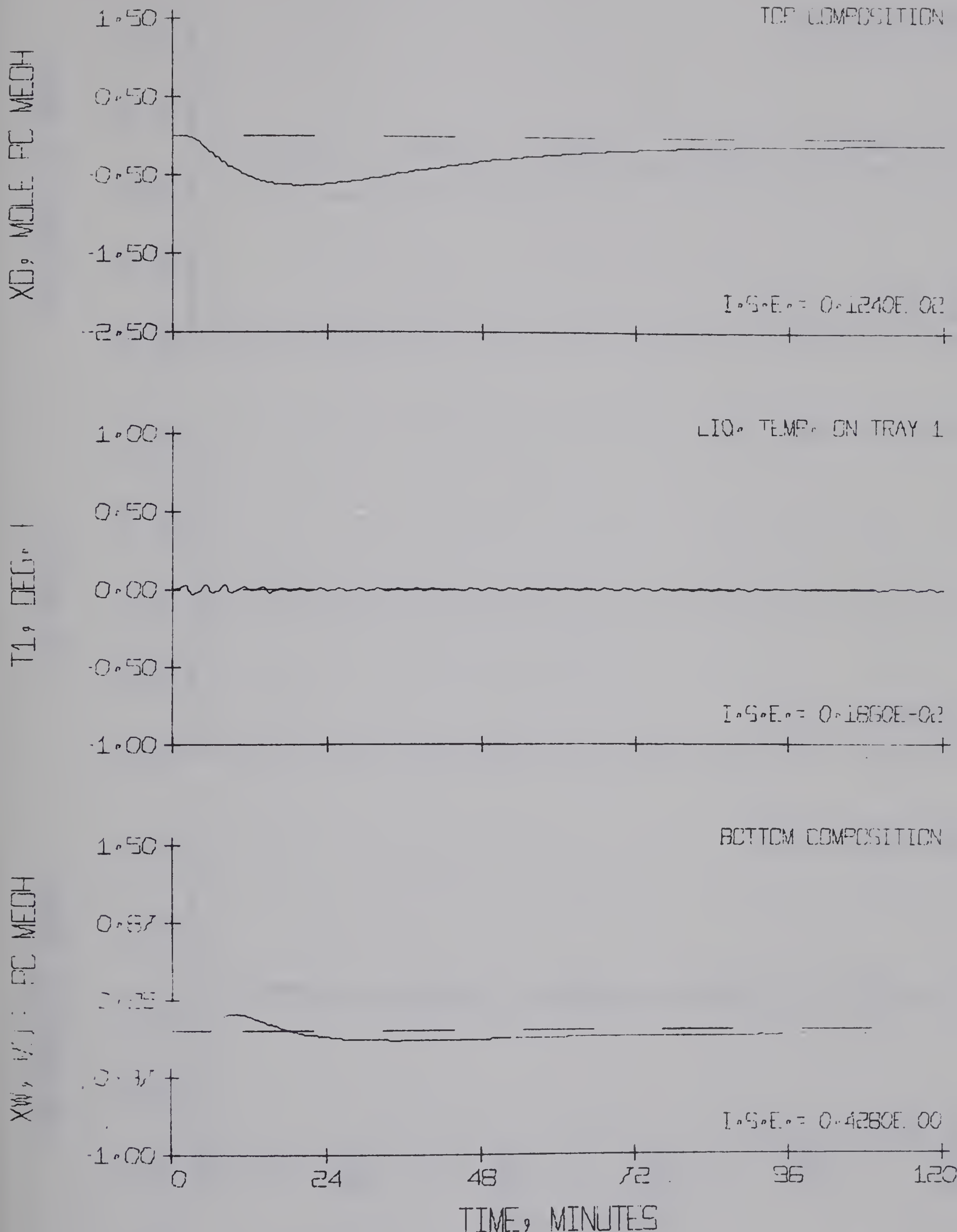


Figure 6.4-44 Feedforward Plus Feedback Control of the Liquid Temperature on Tray 1 by Manipulation of Steam Flow - PI Feedback Controller, τ_I = 10.0 min. (University of Alberta Column)

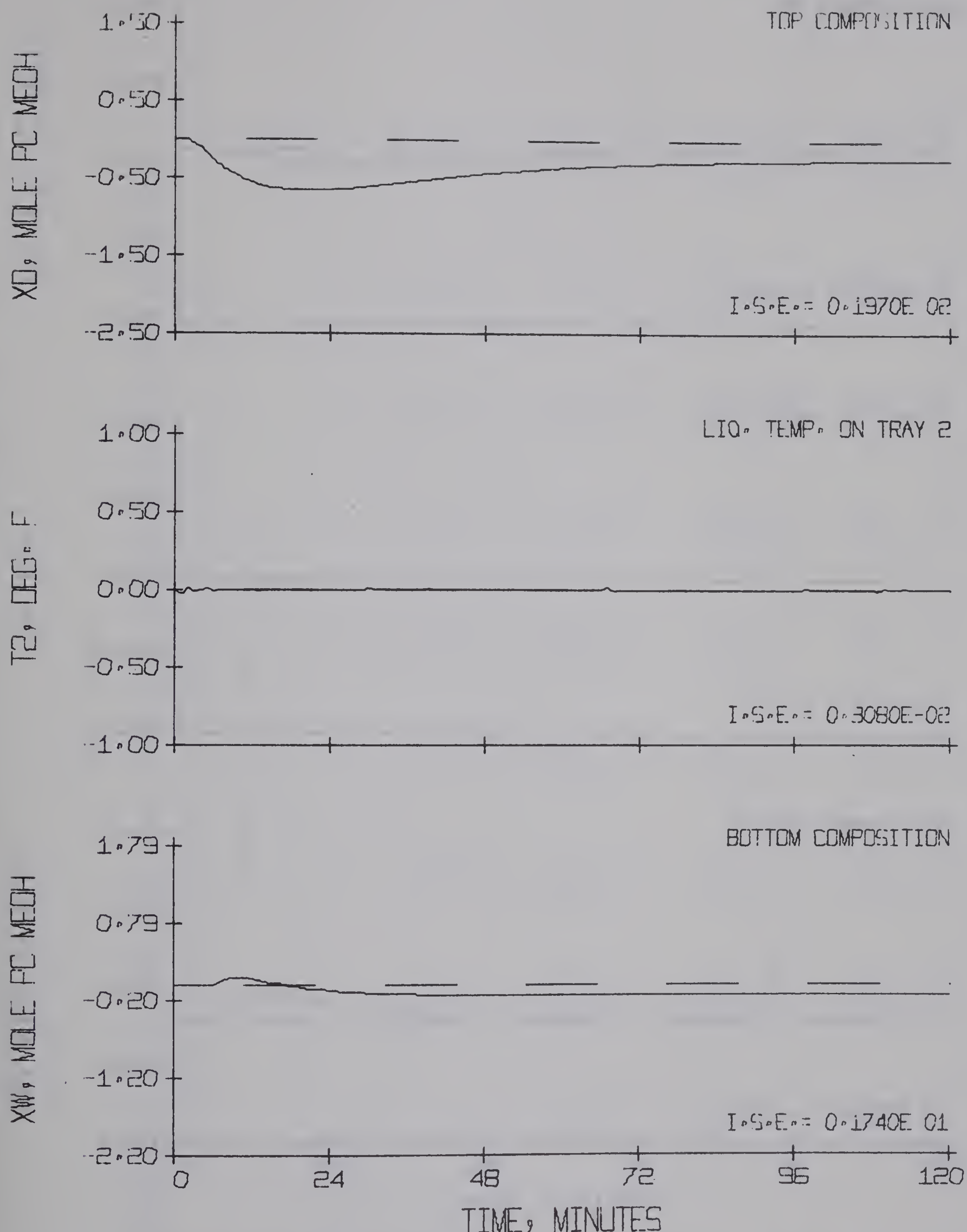


Figure 6.4-45 Feedforward Plus Feedback Control of the Liquid Temperature on Tray 2 by Manipulation of Steam Flow - PI Feedback Controller, τ_I = 10.0 min. (University of Alberta Column)

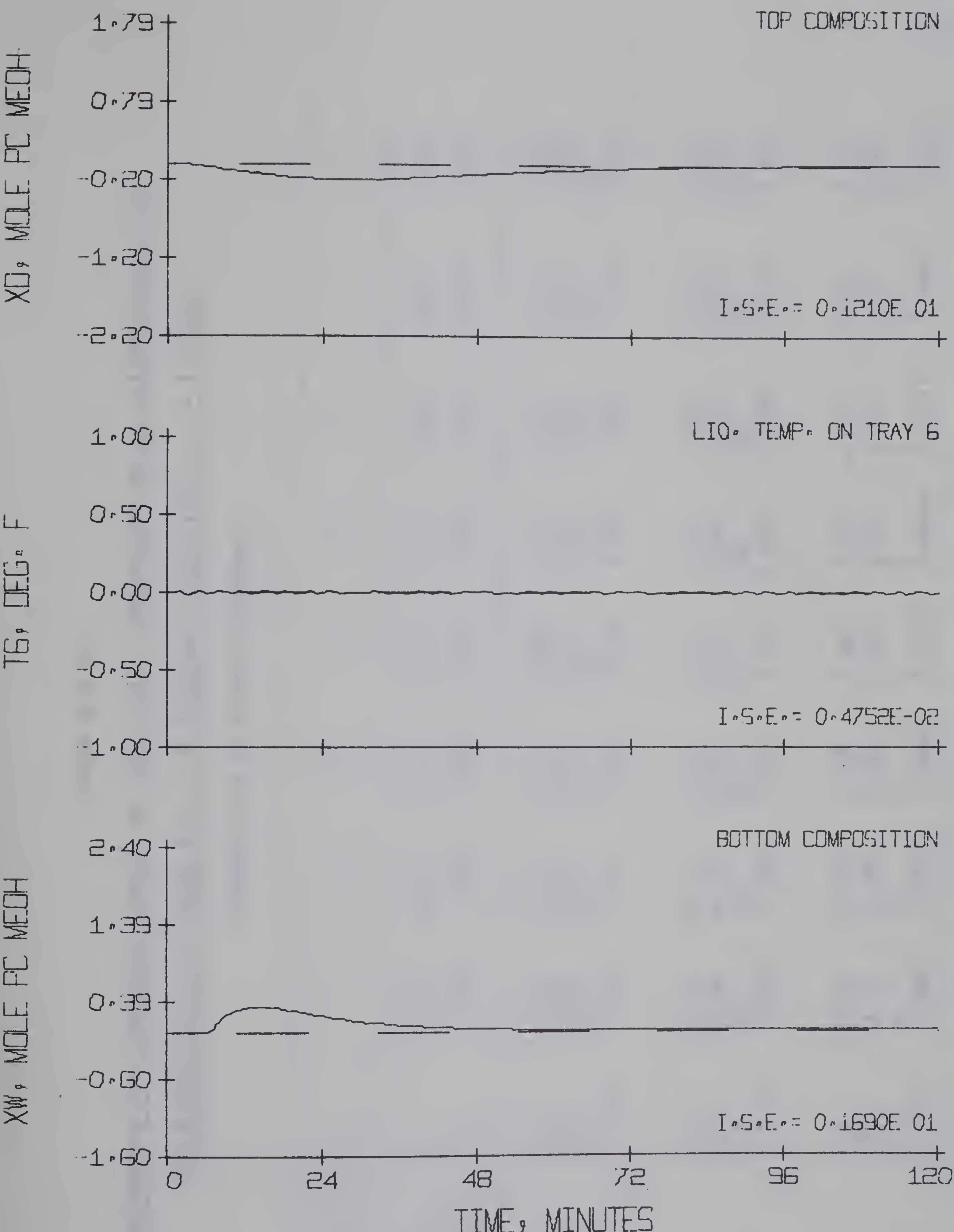


Figure 6.4-46 Feedforward Plus Feedback Control of the Liquid Temperature on Tray 6 by Manipulation of Steam Flow - PI Feedback Controller, τ_I = 10.0 min. (University of Alberta Column)

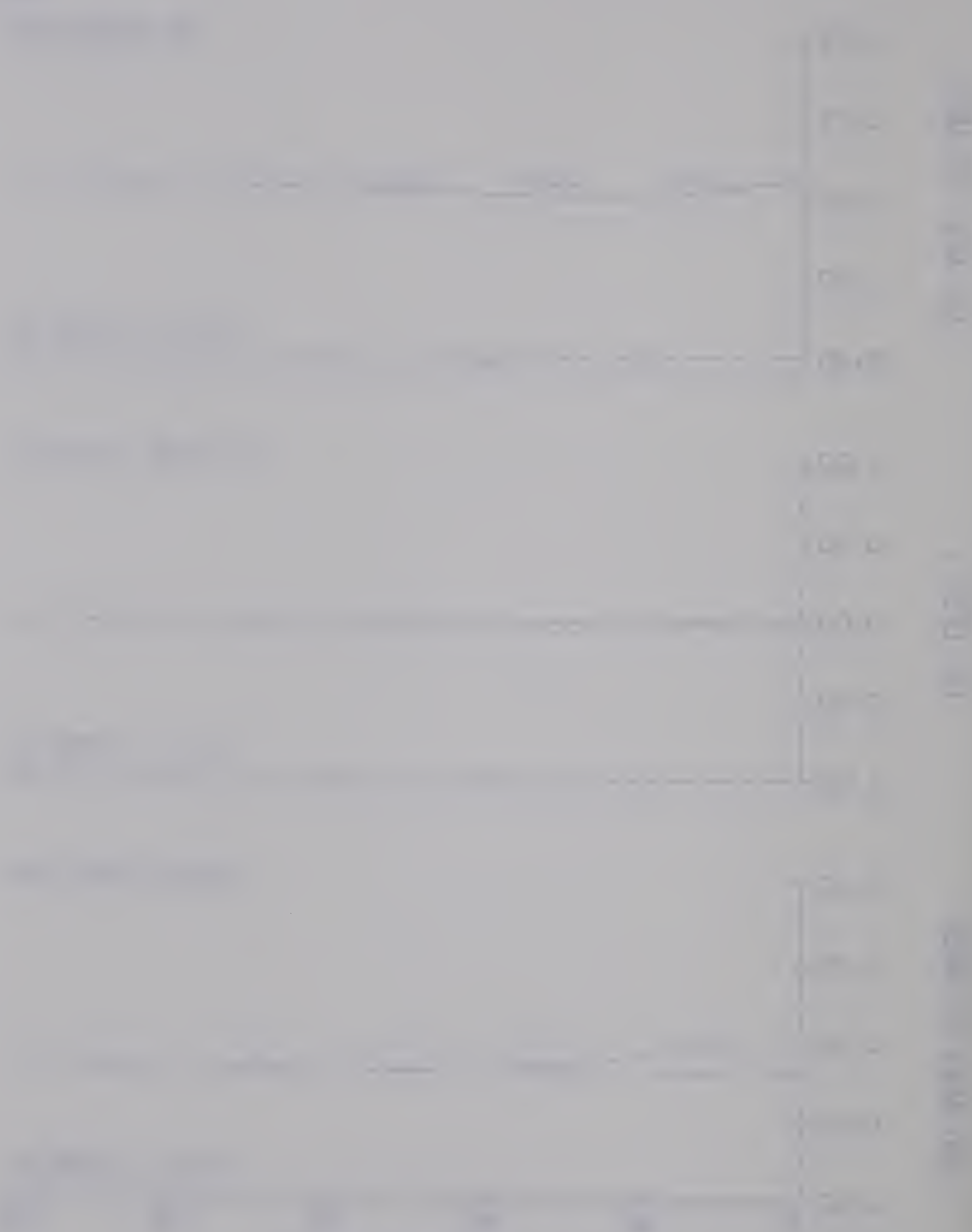


Table 6.4-24

Feedforward Plus Feedback Control of the Liquid Temperature on an Intermediate Tray

by Manipulation of Steam Flow - PI Feedback Controller, τ_I = 1.0 min.

(University of Alberta Column)

Control Tray		1	2	3	4	5	6	7	8
Optimum controller settings	K_c	25.0	20.0	22.0	26.0	28.0	30.0	34.0	35.0
	K_{FF}	0.267	0.282	0.296	0.291	0.266	0.258	0.206	0.201
X_D	M.D.	-0.63	-0.67	-0.75	-0.69	0.39	-0.20	0.51	0.39
	Off.	-0.08	-0.24	-0.39	-0.34	-0.07	0.02	0.51	0.39
	S.T.	102.	99.	91.	90.	110.	114.	87.	85.
	I.S.E.	12.43	19.71	32.57	25.94	5.578	1.208	17.14	8.673
X_W	M.D.	0.14	-0.14	-0.22	-0.19	0.17	0.34	0.51	0.38
	Off.	-0.04	-0.13	-0.22	-0.19	-0.04	0.02	0.29	0.23
	S.T.	93.	61.	42.	41.	86.	56.	58.	52.
	I.S.E.	0.4281	1.742	4.411	3.175	0.4511	1.690	12.21	7.447
T_i	M.D.	-0.05	0.05	0.00	0.00	0.02	-0.03	0.00	0.00
	Off.	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	S.T.	6.	5.	5.	1.	2.	6.	0.	0.
	I.S.E.	0.0021	0.0030	0.0000	0.0000	0.0006	0.0051	0.0001	0.0000

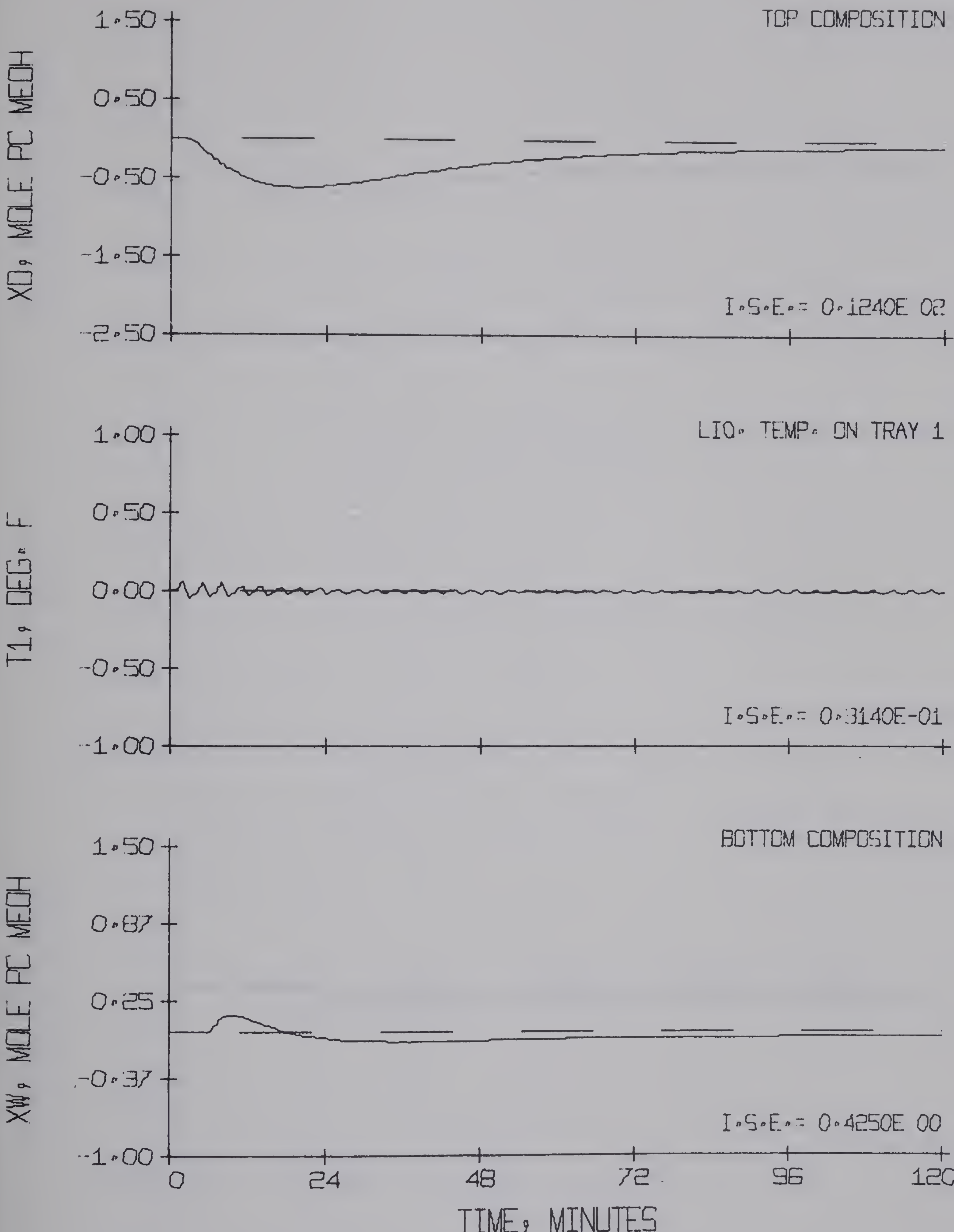


Figure 6.4-47 Feedforward Plus Feedback Control of the Liquid Temperature on Tray 1 by Manipulation of Steam Flow - PI Feedback Controller, τ_I = 1.0 min. (University of Alberta Column)

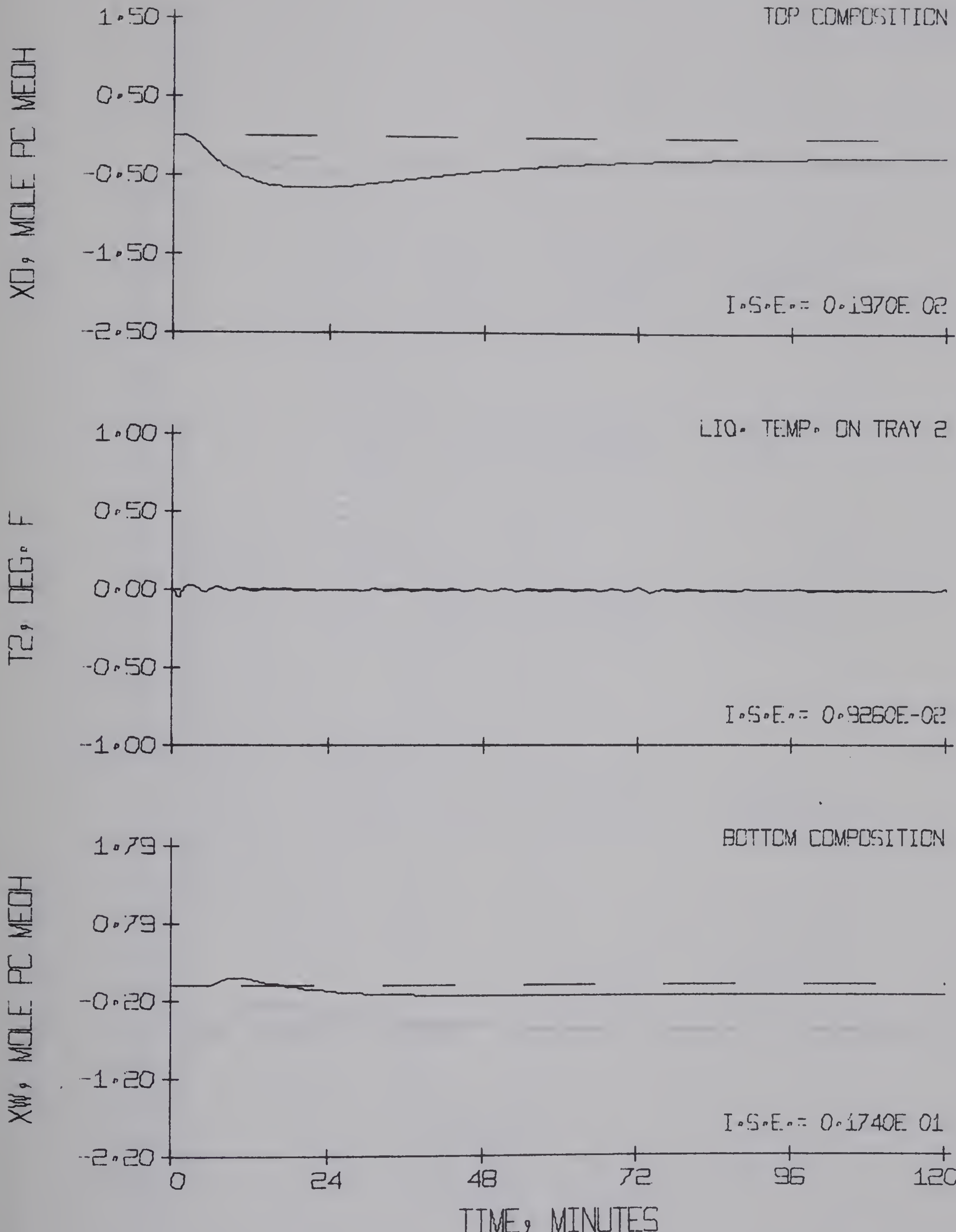


Figure 6.4-48 Feedforward Plus Feedback Control of the Liquid Temperature on Tray 2 by Manipulation of Steam Flow - PI Feedback Controller, τ_I = 1.0 min. (University of Alberta Column)

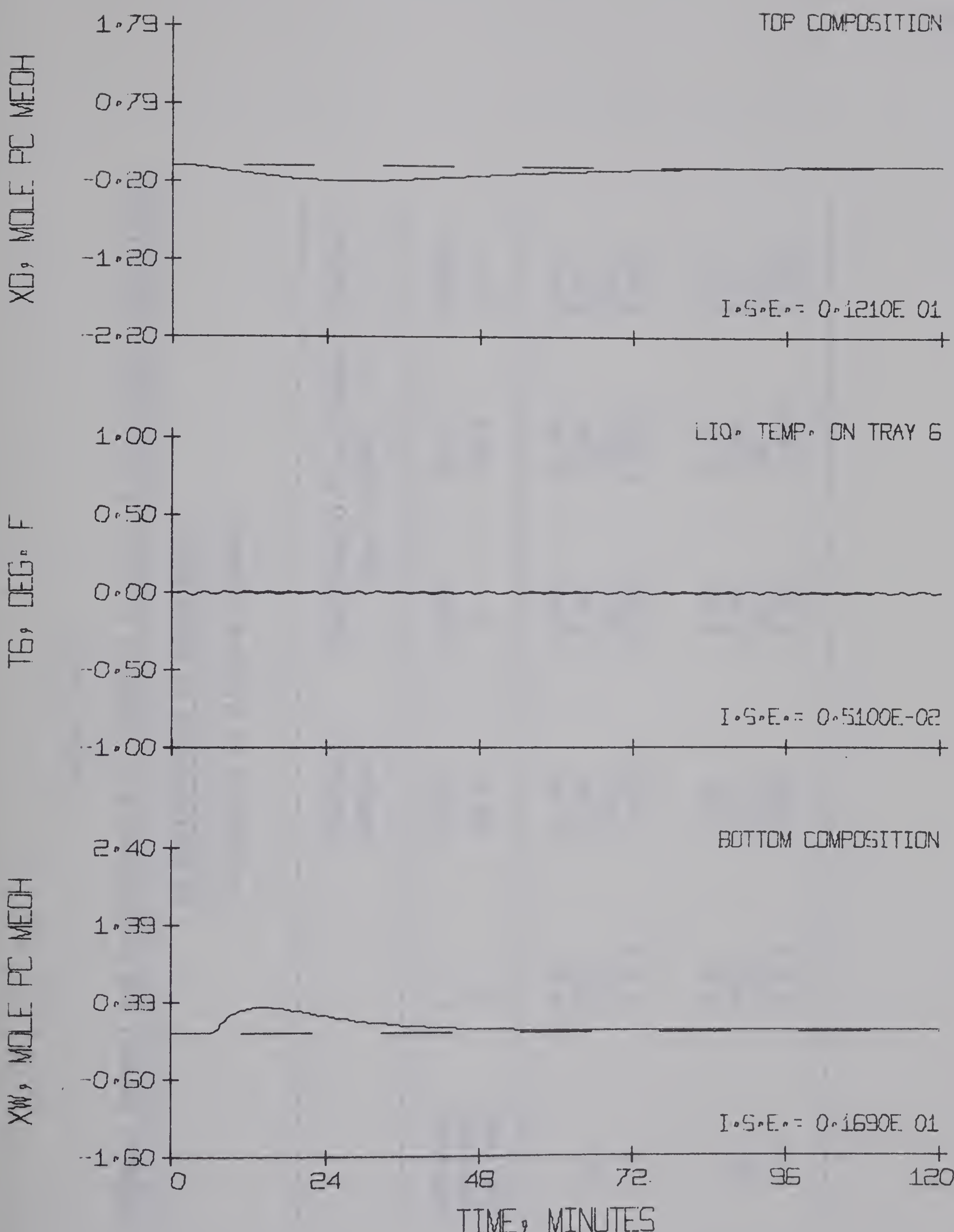


Figure 6.4-49 Feedforward Plus Feedback Control of the Liquid Temperature on Tray 6 by Manipulation of Steam Flow - PI Feedback Controller, τ_I = 1.0 min. (University of Alberta Column)

Table 6.4-25

Feedback Control and Feedforward Plus Feedback Control of Top Product Composition

by Manipulation of Steam Flow

(University of Alberta Column)

		Feedback Control	Feedforward Plus Feedback Control $K_{FF} = 0.260$		
Optimum controller settings	K_c	-0.65	-0.45	-0.31	-0.0003
	τ_I	28.0	∞	10.0	1.0
X_D	M.D.	-2.50	-2.23	-2.32	-3.15
	Off.	0.00	0.00	0.00	0.00
	S.T.	102.	95.	96.	110.
	I.S.E.	0.6255	0.2428	0.5313	3.865
X_W	M.D.	0.57	0.46	0.47	0.25
	Off.	0.01	0.01	0.01	0.01
	S.T.	68.	62.	64.	105.
	I.S.E.	4.984	3.077	3.803	0.6306

Table 6.4-26

Feedback Control and Feedforward Plus Feedback Control of Bottom Product Composition

by Manipulation of Steam Flow

(University of Alberta Column)

		Feedback Control	Feedforward Plus Feedback Control $K_{FF} = 0.260$		
Optimum controller settings	K_c	-0.20	-0.13	-0.05	-0.0035
	τ_I	28.0	∞	10.0	1.0
X_D	M.D.	-0.83	-0.47	-0.48	-0.41
	Off.	-0.01	-0.01	-0.01	-0.01
	S.T.	102.	61.	99.	102.
	I.S.E.	5.000	7.110	7.828	4.636
X_W	M.D.	0.77	1.39	1.38	1.40
	Off.	0.00	0.00	0.00	0.00
	S.T.	65.	61.	62.	63.
	I.S.E.	7.240	0.1694	0.2960	0.330

6.5 Comparison of Different Methods of Locating the "Optimum" Control Point

Five different methods for selecting the tray location for temperature (or composition) control of a distillation column have been proposed as described earlier in the Literature Survey section. In summary form, the methods are the following:

(i) Bertrand and Jones method ÷ The control point should be located at the place of maximum temperature (or concentration) gradient in the column which has the least hydrodynamic delay. This method is primarily a refinement of the method suggested by Boyd (17) and Pyle (57).

(ii) Uitti method ÷ The control point should be located where the temperature (or concentration) change is greatest for a given change in the overhead product purity as the result of a disturbance to the column.

(iii) Wood method ÷ This method specifies the control tray to be that tray where if the temperature (or composition) of the liquid on this tray is kept constant will give a minimum steady-state offset in the overhead or the bottom product composition.

(iv) Rosenbrock method ÷ The control tray should have the greatest effect in maintaining constant conditions throughout the column

(v) Williams method ÷ For the control by manipulation of reflux flow, measurement of the liquid composition on the top tray is recommended, while if steam flow is used as the manipulative variable, locating the sensor on the bottom tray is preferable.

These methods have been utilized where data exist to predict the control tray locations for the two columns under investigation. The sensor locations have then been compared with the locations predicted by the simulation results. The sensor location determined by the latter method is based mainly on the tray where if the liquid temperature (or composition) on this tray is kept constant, will give a minimum value of the I.S.E. performance for the top or the bottom product composition.

6.5.1 Predictions of the Optimum Control Tray Locations for the University of Delaware Column

To determine the control tray location by the Bertrand and Jones method, the steady-state concentration profile has been plotted. It can be seen from Figure 6.5-1 that the composition gradient is steepest at trays 9 and 3.

The necessary calculations used to determine the control tray location by Rosenbrock's method appear in Appendix E.1, whereas the optimum control tray location predicted by the simulation results is determined by examining the results of section 6.4-1.

6.5.2 Predictions of the Optimum Control Tray Locations for the University of Alberta Distillation Column

The basis for the selection of control tray location using the Bertrand and Jones method is illustrated in Figure 6.5-2. It can be seen that the temperature profile is steepest at tray 5 in the rectifying section and at tray 3 in the stripping section.

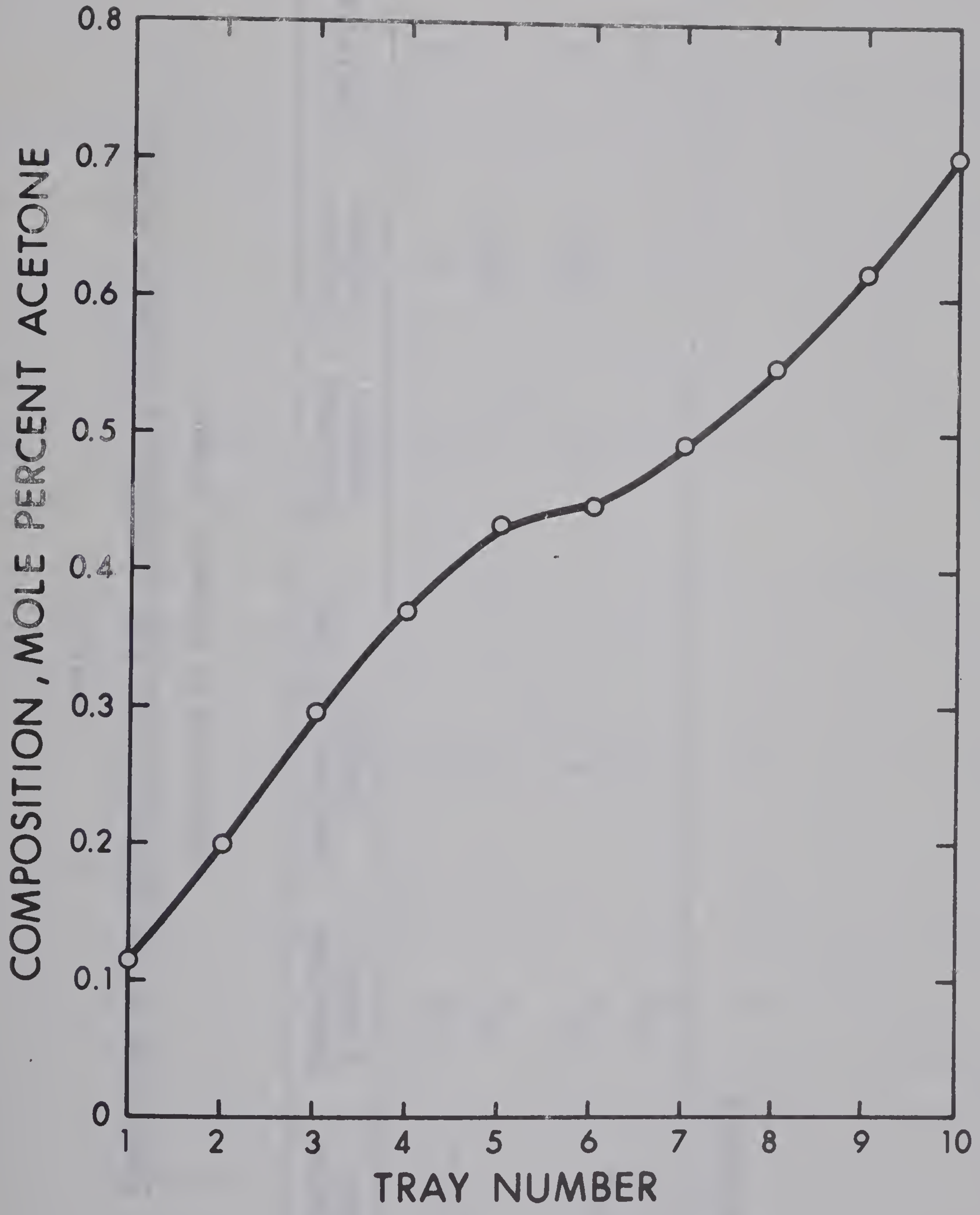


Figure 6.5-1 Composition Profile of the University of Delaware Column

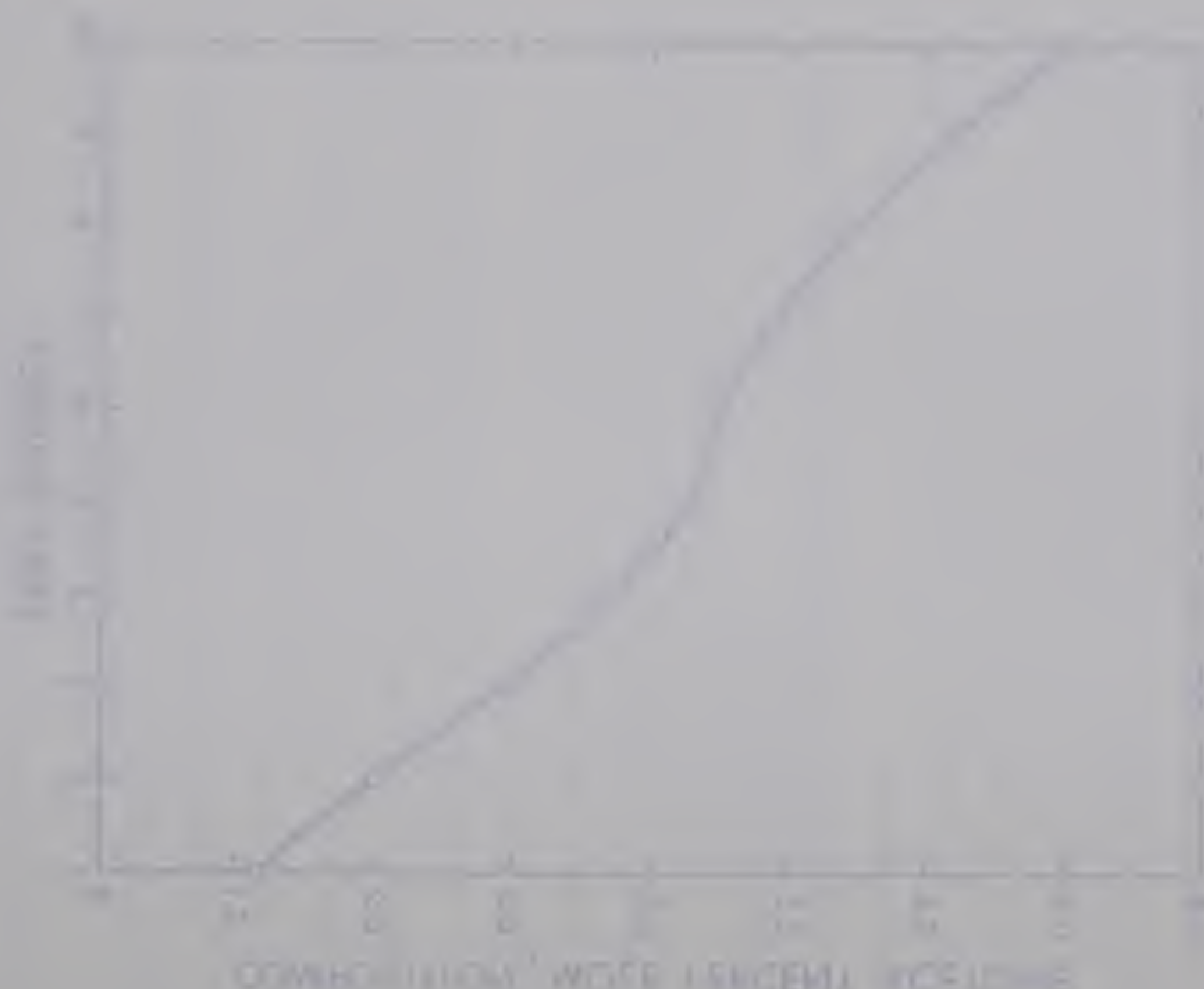

COMPOSITION, MOLE PERCENT ACETONE

Table 6.5-1

Predictions of the Optimum Control Tray Locations by Different Methods

(University of Delaware Column)

Manipulative Variable	Controlled Product	Bertrand and Jones Method	Rosenbrock Method	Williams Method	Simulations
Reflux flow	X_D	9	9	9	9
	X_W	3	1	N/A*	1
Steam flow	X_D	9	9	N/A*	9
	X_W	3	3	1	3

*not applicable

To specify the control tray location by the methods of Uitti and Wood, tests were performed on the actual column to obtain steady-state data.

To obtain the data necessary to apply Uitti's method, the reflux flow was varied, and for each particular reflux rate, the temperature of the liquid on all trays was recorded, and the temperature variations on each tray can be calculated. Figure 6.5-3 shows the amount that the liquid temperature has changed on any tray when the product quality has varied. It is apparent from Figure 6.5-3 that trays 6 and 2 exhibited the greatest changes in temperature for a given change in product purity.

To select the optimum control tray location using Wood's method, if reflux flow is used as the manipulative variable, tests were performed at different reflux flow rates with the steam flow rate held constant. In order to evaluate the effect of feed flow rate variations, a change of feed flow rate from 50 per cent to 40 per cent feed flow (on the feed flow recording chart) was used. Figure 6.5-4 is a plot of the liquid temperature on trays 6, 7 and 8 versus top product composition at varying feed flow rates. It can be seen from Figure 6.5-4 that if tray 8 is the control tray and the initial overhead product composition is 95.50 per cent methanol, holding the liquid temperature on this tray constant would result in overhead product containing 95.57 per cent methanol when the feed flow rate decreases from 50 per cent to 40 per cent. Tray 8 should be used as control tray if top product com-

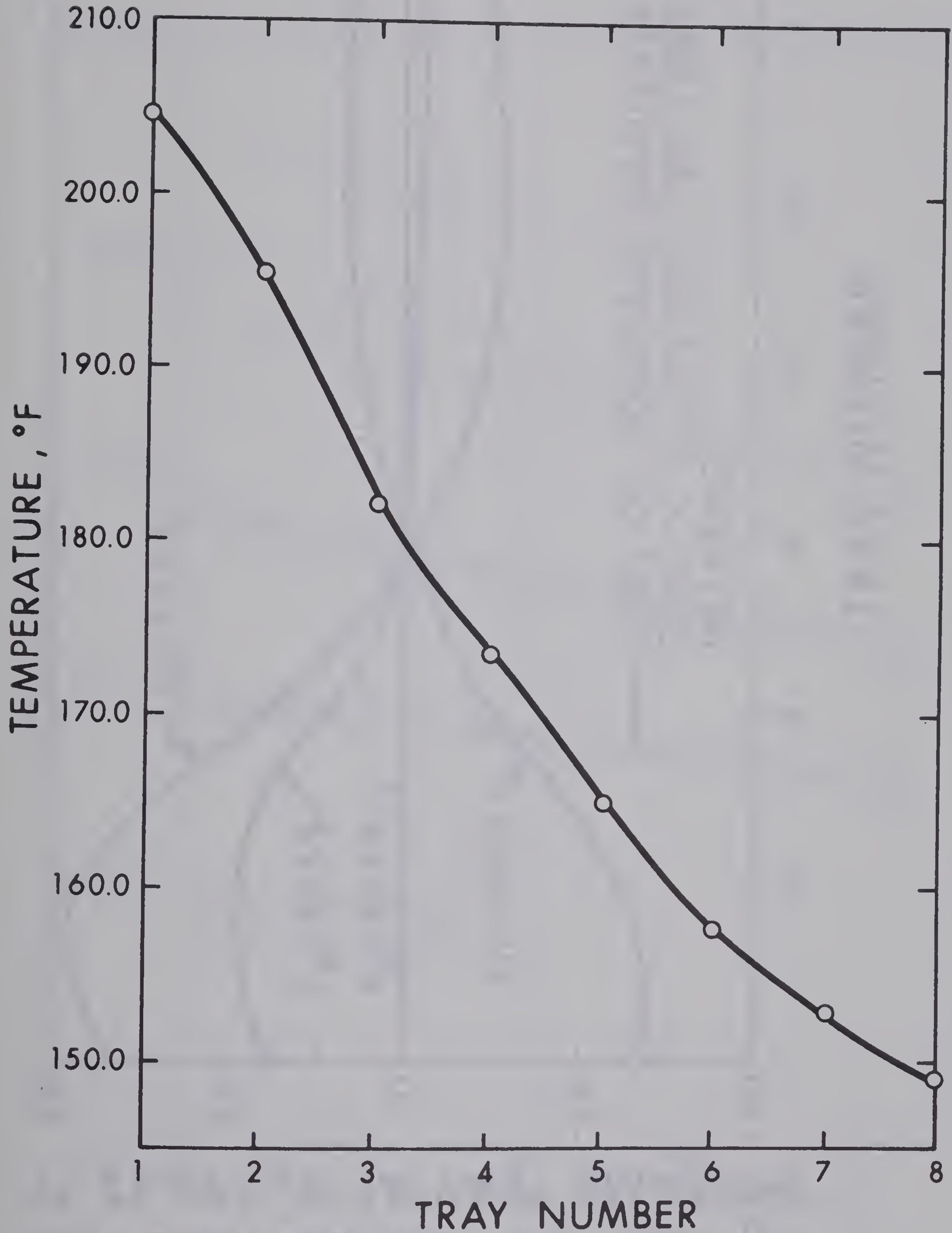
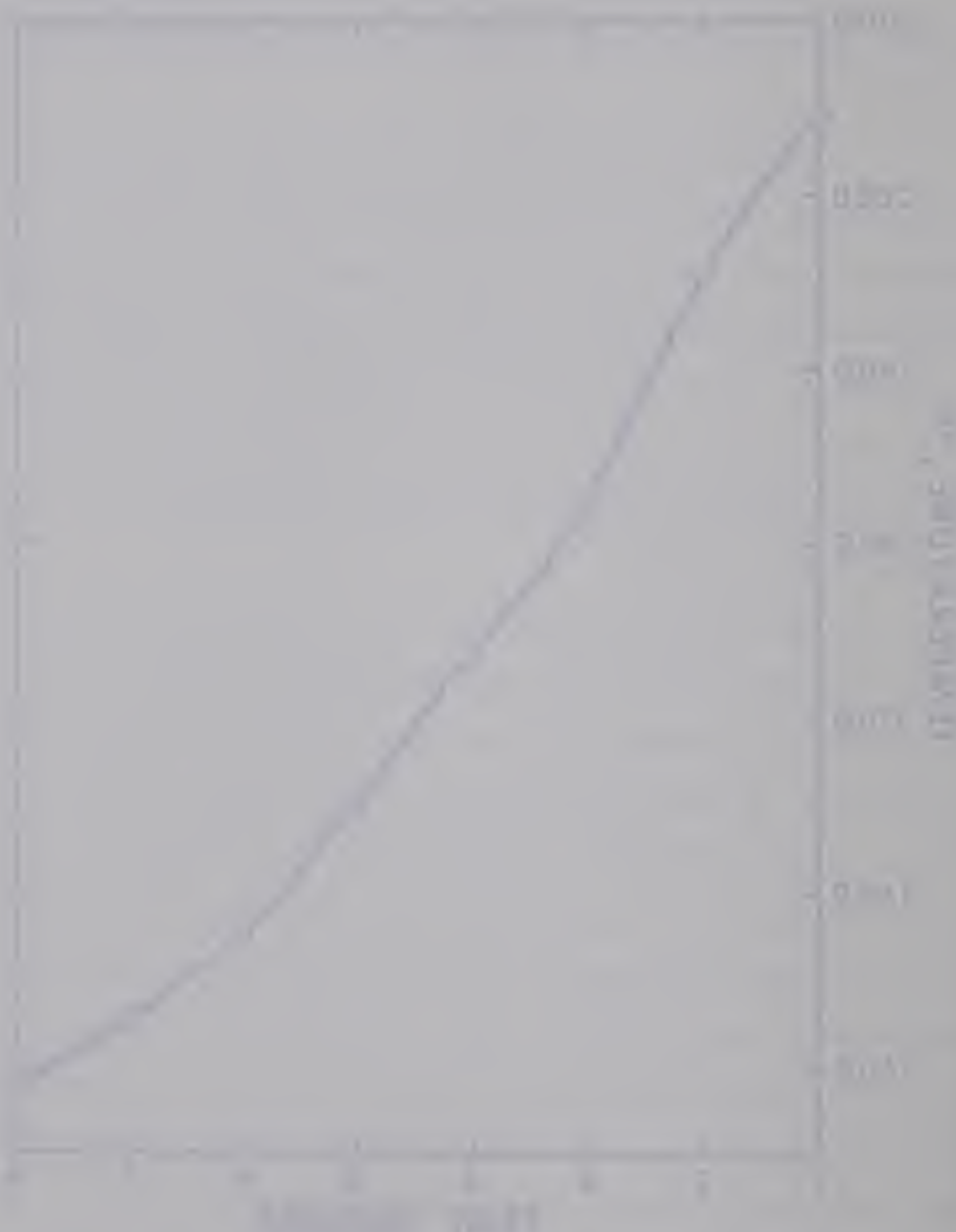


Figure 6.5-2 Temperature Profile of the University of Alberta Column



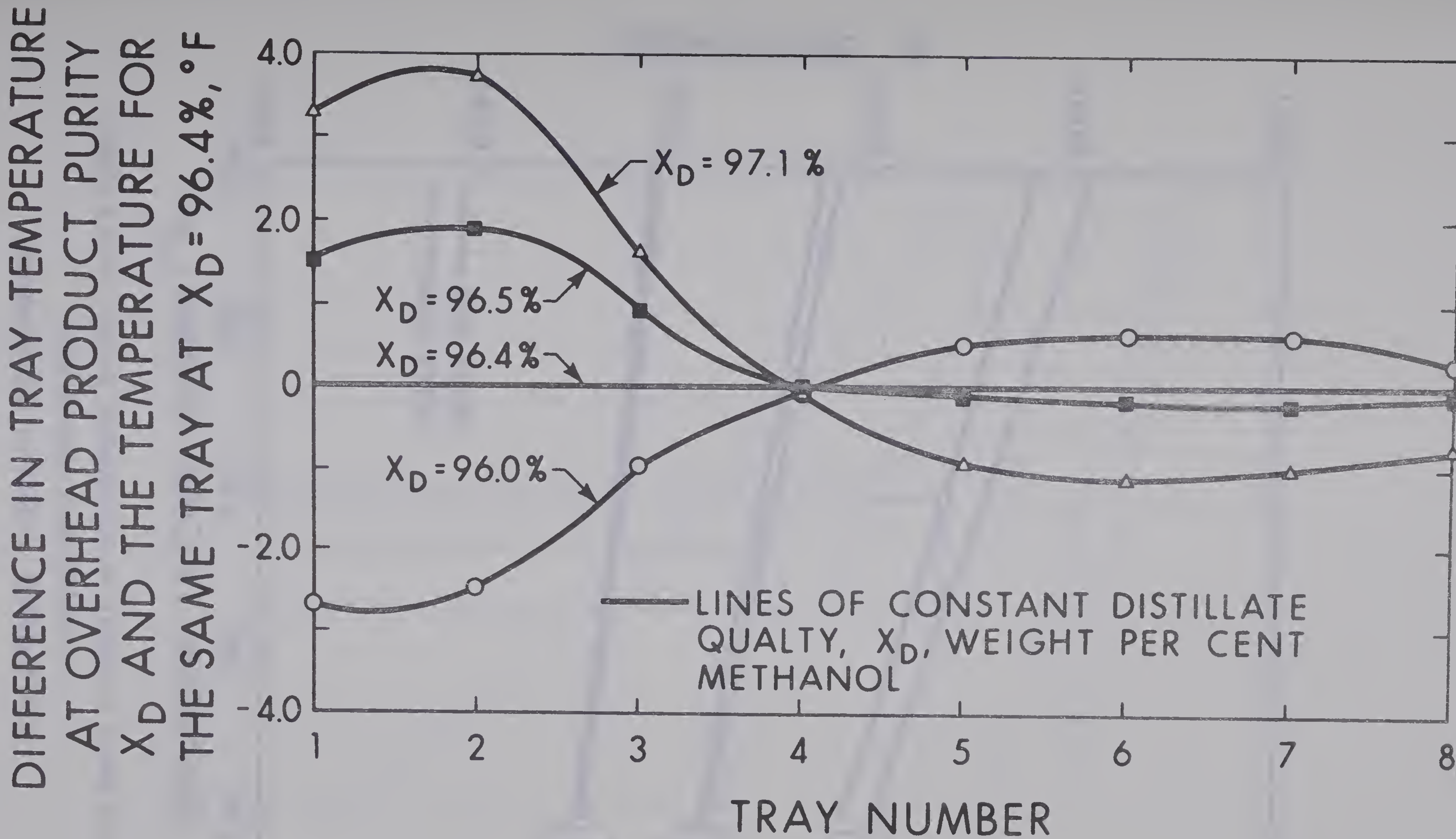


Figure 6.5-3 Change of the Liquid Temperature on Intermediate Trays with Top Product Composition

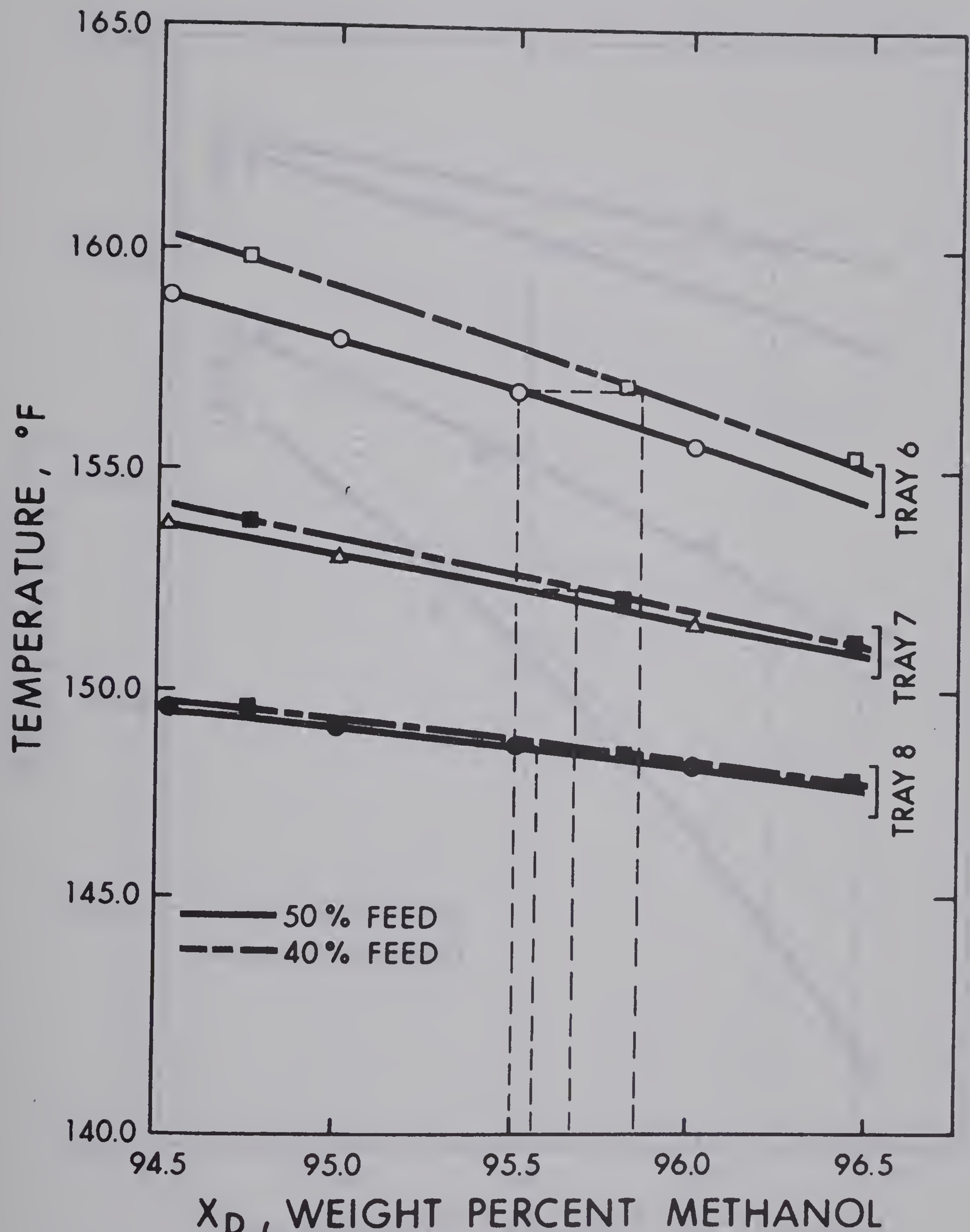
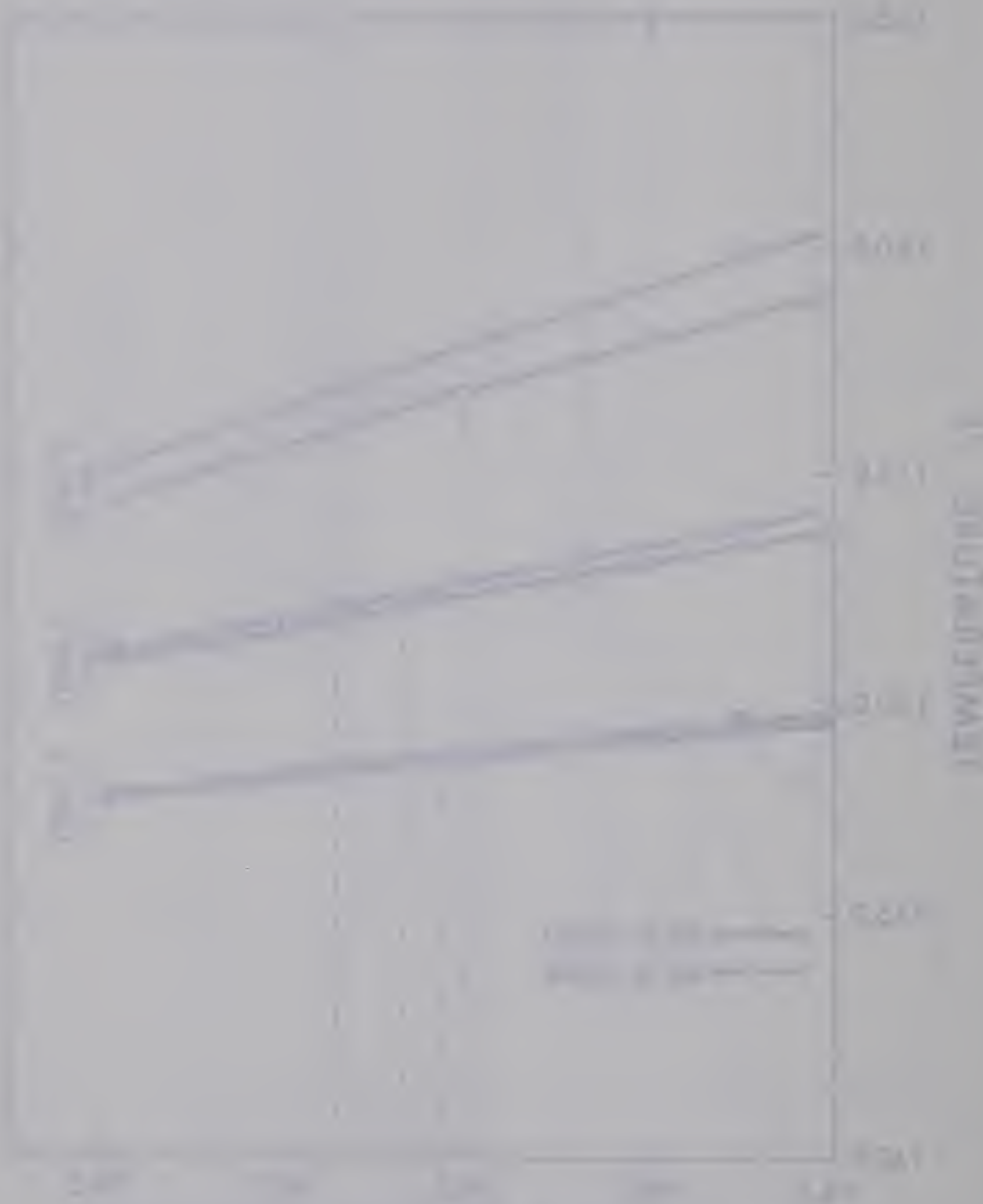


Figure 6.5-4 Liquid Temperature on Trays 6, 7 and 8 vs. Top Product Composition (Manipulative Variable: Reflux Flow)



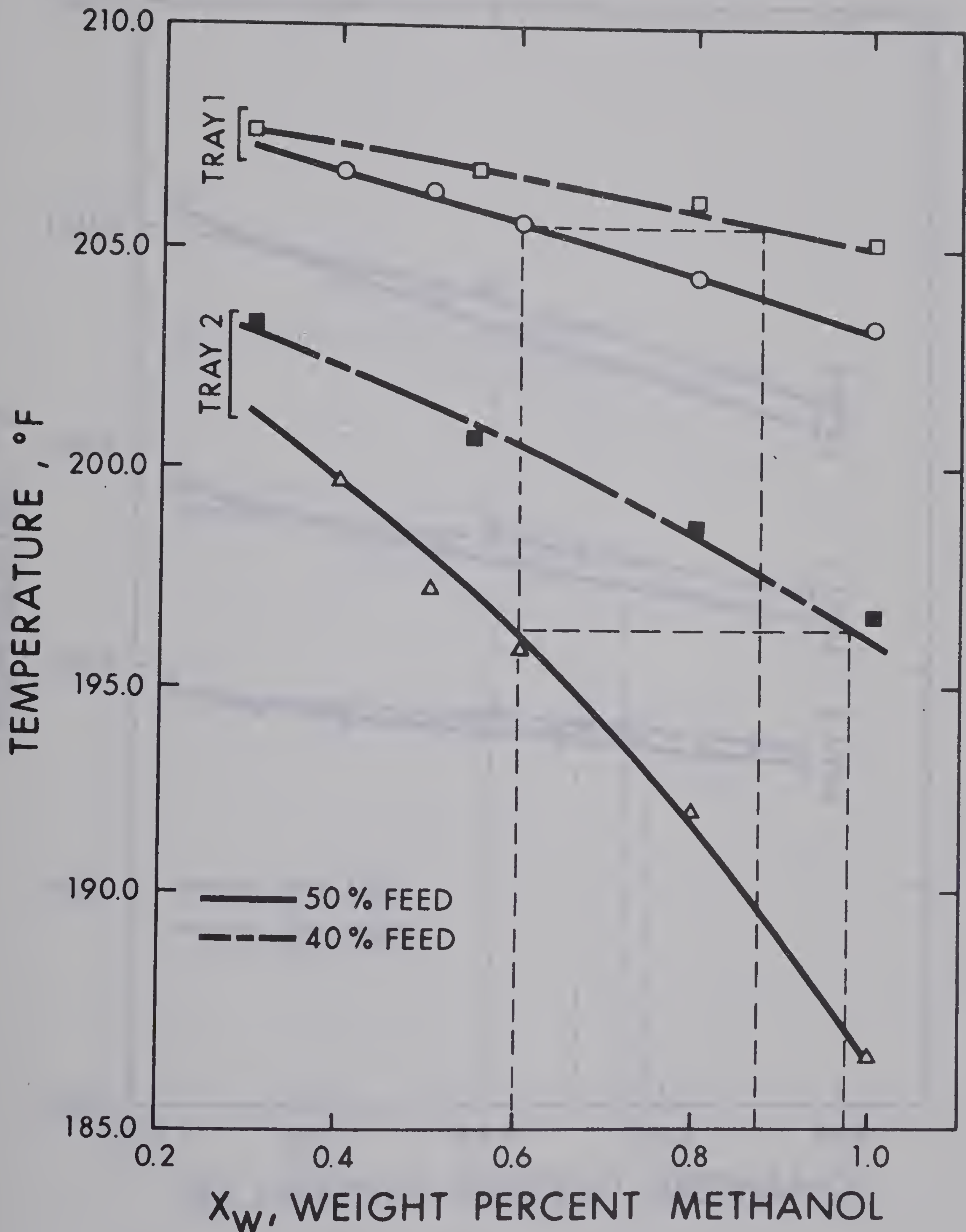


Figure 6.5-5 Liquid Temperature on Trays 1 and 2 vs. Bottom Product Composition (Manipulative Variable: Reflux Flow)

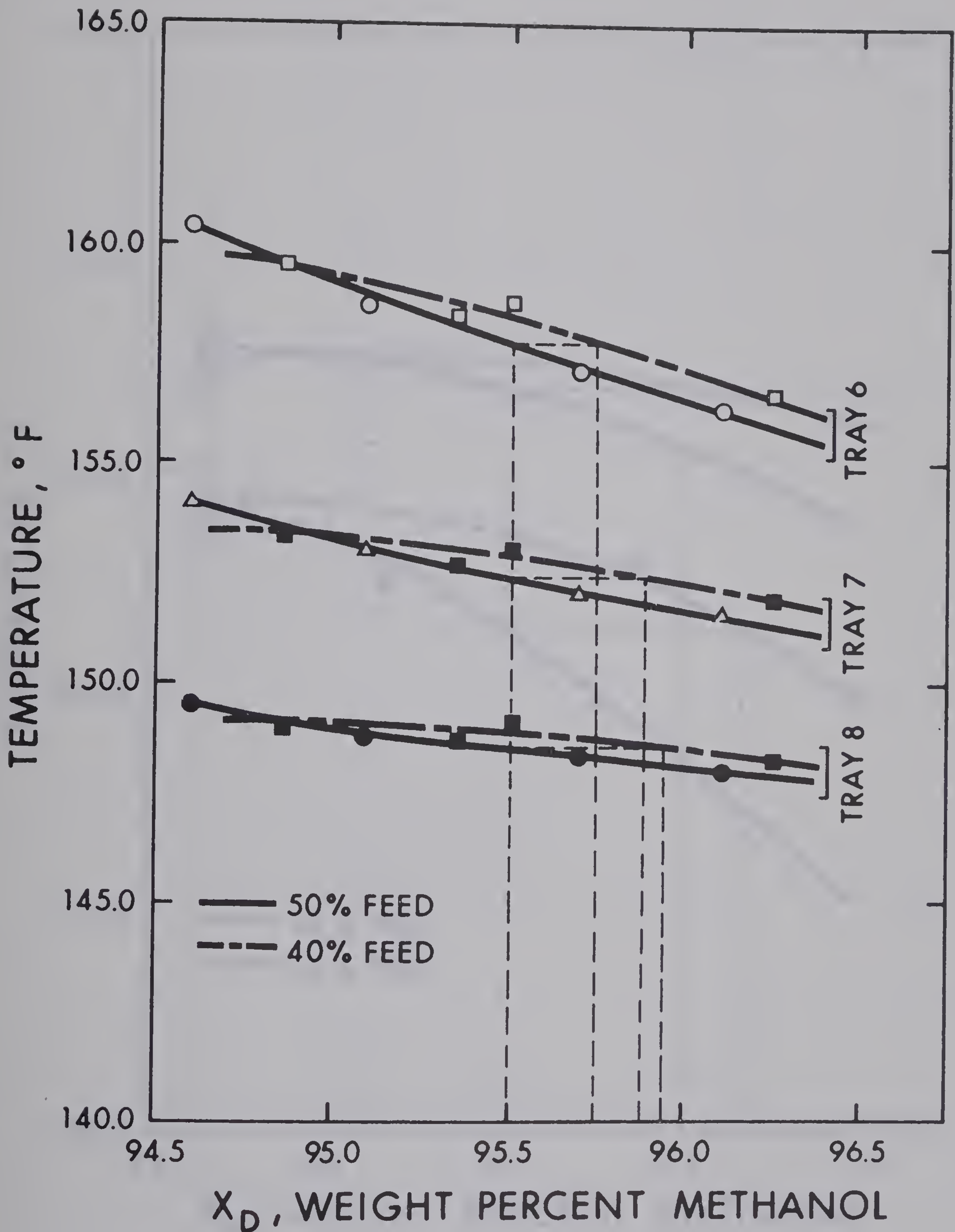


Figure 6.5-6 Liquid Temperature on Trays 6, 7 and 8 vs.
Top Product Composition
(Manipulative Variable: Steam Flow)

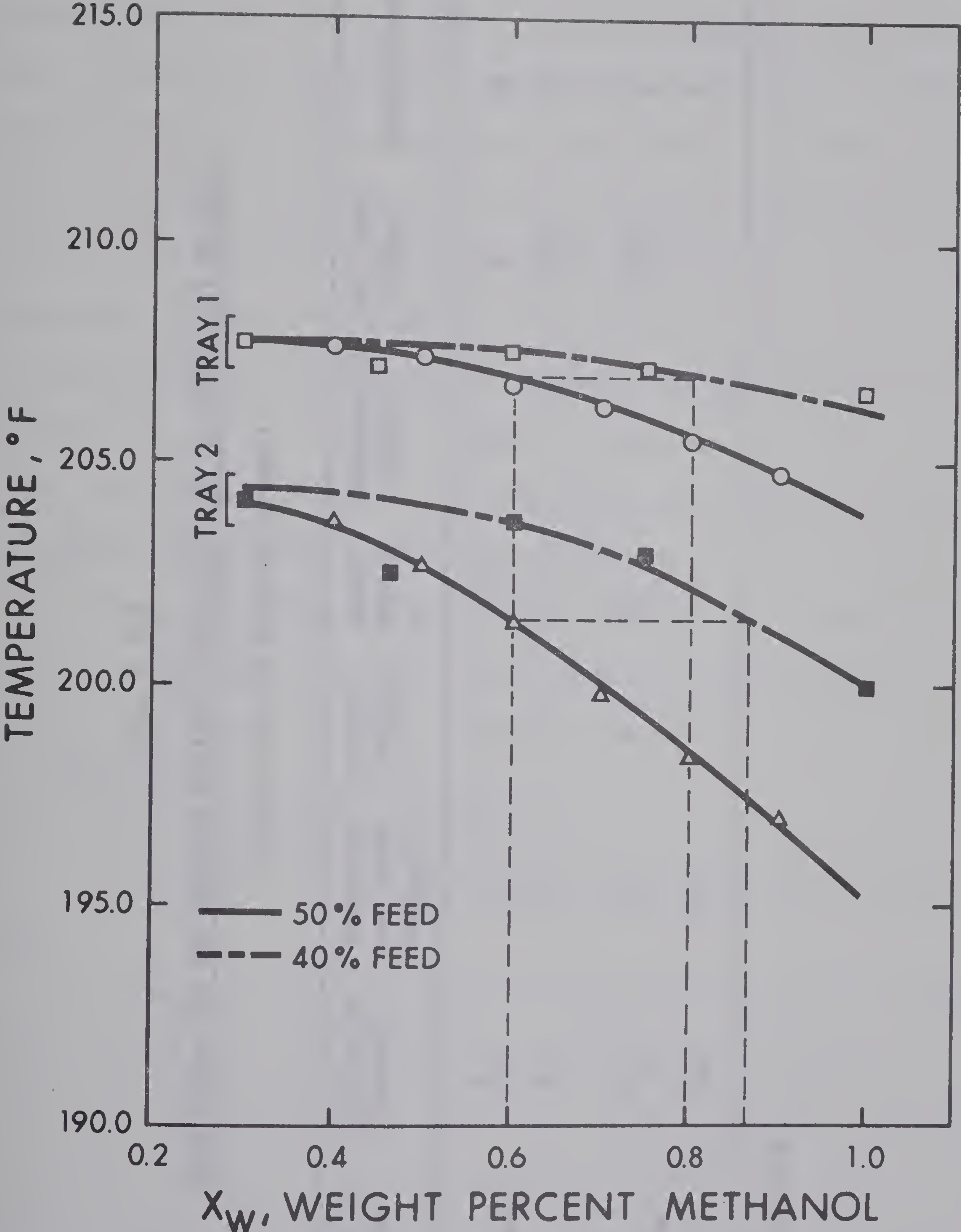


Figure 6.5-7 Liquid Temperature on Trays 1 and 2 vs. Bottom Product Composition (Manipulative Variable: Steam Flow)

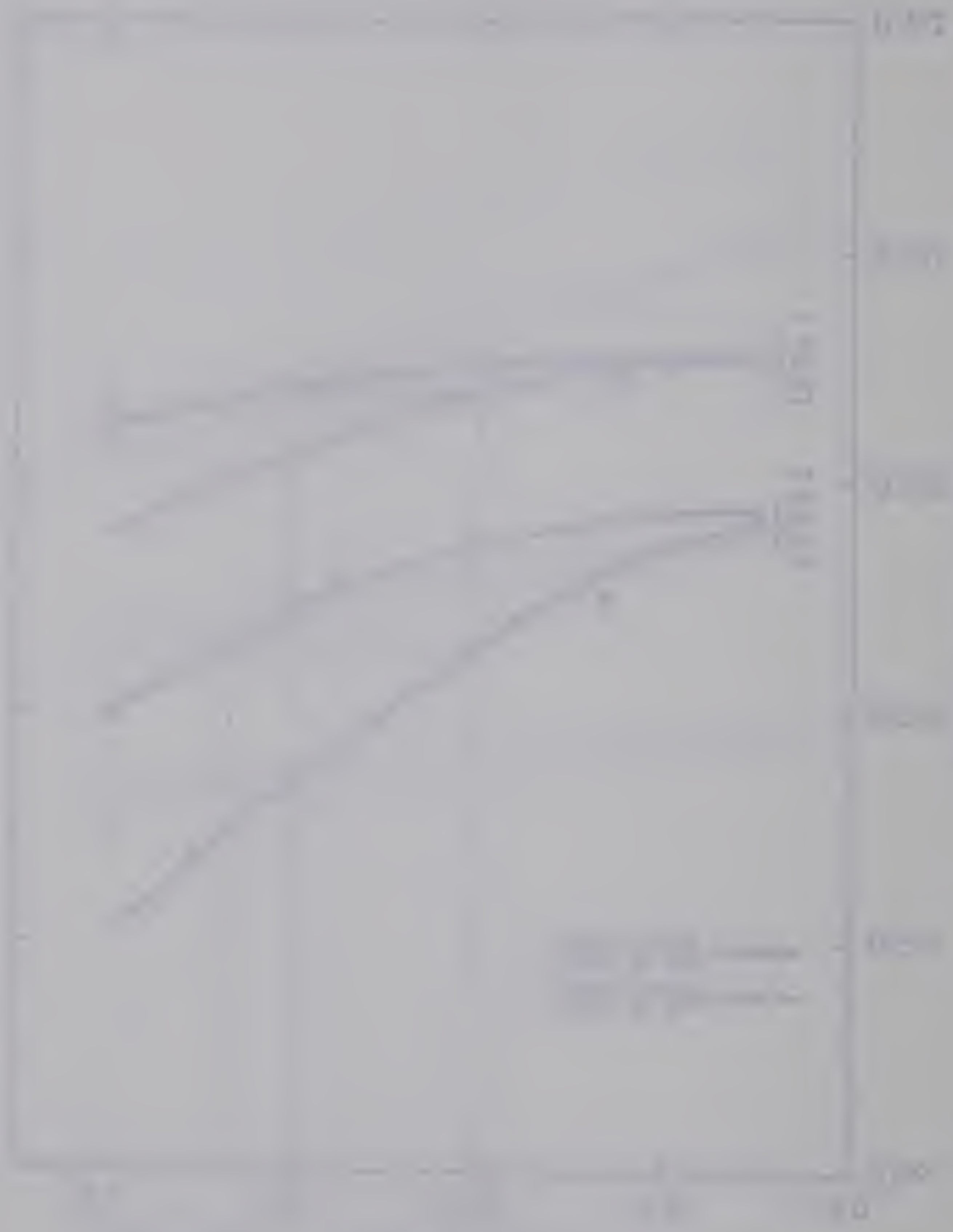


Table 6.5-2

Predictions of the Optimum Control Tray Locations by Different Methods

(University of Alberta Column)

Manipulative Variable	Controlled Product	Bertrand and Jones Method	Uitti Method	Wood Method	Rosenbrock Method	Williams Method	Simulations
Reflux flow	X_D	5	6	8	6	8	8
	X_W	3	2	1	2	N/A*	1
Steam flow	X_D	5	6	6	6	N/A*	6
	X_W	3	2	1	2	1	1

*not applicable

position is to be maintained constant and reflux flow is used as the manipulative variable since holding the liquid temperature on other trays, for instance tray 6 and 7 constant would result in a higher steady-state offset in the top product composition. If bottom product composition is desired and reflux flow is used as the manipulative variable, tray 1 should be employed as the control tray, as shown in Figure 6.5-5. Other conclusions for the case where steam flow is used as the manipulative variable can be reached by examining Figures 6.5-6 and 6.5-7.

Appendix E.2 outlines the necessary calculations to locate the optimum control tray by Rosenbrock's method.

The predictions of control tray location from simulation results are obtained by examining the results of section 6.4-2.

6.6 Discussion

6.6.1 Discussion of Simulation Results

An analysis of the simulation results reveal the following points.

(i) Effect of the selection of the order of the transfer functions representing the dynamics of the column ÷ As shown in Figures 6.4-1 and 6.4-2, there is practically no transient period during which the liquid composition on trays 7 and 9 would be off-specification. This is probably the result of the approximation of the dynamics of the liquid composition on trays 7 and 9 to changes in reflux flow by a simple first order transfer function without time delay. The addition of an-

other first order transfer function representing the dynamics of the measuring element in the control loop has essentially no de-stabilizing effect on the column responses. However, it should be kept in mind that the selection of the order of the transfer function is rather arbitrary, and consequently, use of the simplest order of the transfer function might result in the conclusion that the column is inherently stable which in fact, it is not.

(ii) Effect of the presence of time delay in the control loop ÷ The impact of the presence of a pure time delay in the control loop can be seen from the results of both distillation columns under investigation when reflux flow is used as the manipulative variable. This can be appreciated by examining Table 6.4-1 which summarizes some of the results obtained using data from the University of Delaware column. Comparing the performance of this column when tray 1 or 3 is used as control tray with the performance of the column when the liquid composition on tray 7 or 9 is controlled shows that due to a time delay of 0.5 minutes and 1.0 minutes in the control loop for composition control using trays 3 and 1 respectively, the control is not as satisfactory as that possible using tray 7 or 9 where no time delay is present.

The simulations using data from the University of Alberta distillation column also show this effect. This can be seen by studying Table 6.4-16 or Figures 6.4-26, 6.4-27 and 6.4-28. Figures 6.4-26 and 6.4-27 show the responses of the column with feedback control of the liquid temperature on trays 6 and 7 respectively. A time delay of 0.5

minutes was present in the temperature control loop of tray 6 and a time delay of 0.3 minutes was associated with the control loop of tray 7. These figures should be compared with Figure 6.4-28 which shows the results obtained using as the control tray, tray 8 where no time delay is present. It is obvious that without time delay, the column is inherently stable, as the liquid temperature on tray 8 can be controlled very closely with no sign of oscillation. Locating the sensor on tray 6 or 7 results in slower response because of the exponential lag which hinders the detection of the temperature changes that are occurring and the application of proper corrections. As the size of the time delay increases, the period of oscillation becomes larger. From these results, one may conclude that there would be a deterioration in the responses that would be obtained by locating the sensor on any tray which is situated far down the column where the time delay in the control loop becomes large due to a wide separation between the control point and the reflux flow control valve. (The fluid flow lag was equivalent to 0.27 minutes per plate). Indeed, as anticipated, by examining Table 6.4-16, the transient responses of trays 1, 2 and 3 are not very satisfactory as more oscillatory action is present and the responses are characterized by a long settling time. In addition, due to the phase shift involved in the pure time delay, the presence of any amount of dead time in the process results in a greatly reduced region of controllability as only very small values of proportional constants and large integral time constants can be used

without causing unstability in the column.

(iii) Effect of lag in the reboiler ÷ If steam flow is used as the manipulative variable, in general, the lag in vapor flow between intermediate trays is negligible and the main contribution to the lag involved comes primarily from the reboiler. In some cases, this lag might have a major effect on the controllability of the column. Indeed, simulation of the University of Delaware distillation column which had a lag of 0.5 minutes in the reboiler revealed that control of this column by manipulation of steam rate was difficult. This effect can be seen by comparing Figures 6.4-1 and 6.4-13. Although both transfer functions G_{7R} and G_{7V} are of first order type without time delay, the control of liquid composition on tray 7 by manipulation of reboil vapor rate is not as satisfactory as manipulation of reflux flow. The oscillatory behavior in Figure 6.4-13 is due presumably to the presence of three first order transfer functions describing the dynamics of the process, the measuring element and the reboiler itself. The simulation results showed that use of the boil-up system with the University of Delaware distillation column has a de-stabilizing effect on the control performance.

With the University of Alberta distillation column, due to the fast dynamics of the reboiler, no lag was involved, therefore, from the control point of view, the control of the liquid temperature on an intermediate tray by manipulation of steam flow has a decided advantage over the manipulation of reflux flow, as can be seen from Figures 6.4-26

and 6.4-40. It is obvious that the response of the liquid temperature on tray 6 by manipulation of steam flow is definitely superior to the response by manipulation of reflux flow. In fact, as shown by Table 6.4-21, the liquid temperature on any intermediate tray of this column can be controlled very closely by manipulation of steam flow rate.

(iv) Effects of the dynamics of other elements in the control loop such as the control valve and the measuring element ÷ The addition of the dynamics of these elements in the control loop, in most cases, serves only to cause oscillations in the control responses of the column. To obtain better performance of the column, these elements should have as fast a response as possible. Fortunately, with a distillation column, in most cases, the control valve has a fast response compared with the response of the process, so the major problem remaining is to find a measuring element with a fast response. Consequently, because of the fast dynamics of the thermocouples, temperature control would be preferred over composition control if the composition analyzer has a large measurement lag.

(v) Direct control of top product composition ÷ It is a well known fact that if top product composition is desired, the direct sensing of overhead composition has a distinct advantage over the sensing of the liquid temperature (or composition) on an intermediate tray since no offset would be present in the overhead composition if a conventional proportional plus integral feedback controller is used. However, the controllability of the column should also be considered before any final decision is made concerning the sensor location.

With the University of Alberta distillation column simulation shows that best control can be achieved by sensing top product composition and using reflux flow as the manipulative variable. The increased stability and almost no variation present with measurement of overhead product composition is due to the fact that the capacitance cell can immediately detect the effect of the composition change and then the controller can almost instantaneously make the proper adjustment in the reflux flow rate to compensate. The detection of overhead composition would have allowed very large values of controller constants to be used without endangering the column stability.

However, direct analysis of overhead composition and manipulation of reflux flow for the University of Delaware distillation column will not be as satisfactory. This is due to the measuring lag of the overhead composition analyzer and the presence of 1.0 minutes of time delay in the reflux line. This rendered the column unstable for all but very small values of controller gain.

From a dynamic standpoint, the control of top product composition by manipulation of steam flow is less satisfactory than the control of the liquid temperature (or composition) due to an additional hydraulic lag in the reflux accumulator.

(vi) Direct control of bottom product composition ÷ The control of bottom product composition by manipulation of reflux flow is poor from the dynamic standpoint due to the wide separation of the sensing element and the reflux control valve. The advantage of direct control

of bottom product composition by manipulation of steam flow is not very great since the change in the bottom product composition is smaller than the change in the liquid composition on an intermediate plate, due presumably to the large hold-up of liquid in the reboiler. In addition, this hold-up volume tends to contribute some delay before changes in composition are noticed at the bottom of the column. This control arrangement is not very desirable especially for the University of Alberta distillation column, since the bottom product composition analyzer has a large time delay (2.5 minutes). Here the sampling on an intermediate tray is preferable, if bottom product composition is desired, particularly because the control system is inherently stable and also because of the very small offset in the bottom product composition.

(vii) Effect of adding feedforward control ÷ The simulation results showed that, except for all cases where the control system is inherently stable where feedback control alone is adequate, the transient response of the liquid temperature (or composition) on any intermediate tray under feedforward plus feedback control was superior to conventional feedback control alone, even if the simplest type of feedforward control action is used. Examination of these results demonstrates that with feedforward plus feedback control, in most cases, there has not only been a marked improvement in the I.S.E. of the liquid temperature (or composition) on intermediate tray, but also a reduction in the maximum deviation from the set point and a shorter settling time. The amount of improvement that would result from installation of gain feedforward

control in addition to an existing feedback control loop would likely be significantly greater for an industrial column since the magnitude of time delay present in the control loop would be larger. The simulation results also clearly indicate the disadvantage of using integral action in the feedback loop if feedforward plus feedback control is used. The addition of any amount of integral control in general will increase the maximum deviation, the settling time and the performance index I.S.E. Since in the actual process, integral action would be needed to eliminate any offset due to unknown disturbances and modeling errors in the feedforward controller, this amount of integral control should be reduced to a minimum. Very high value of integral action, for instance τ_1 = 1.0 minutes, might lead to the column behaving in an oscillatory manner, as shown in Figure 6.4-35.

Although the addition of feedforward control to an existing feedback control system of the liquid temperature (or composition) on an intermediate tray improves the control response of the liquid temperature (or composition), it does not necessarily mean that the quality of top or bottom product composition will be improved. In most cases, the effect of feedforward control action on the value of the performance index I.S.E. of either top or bottom product composition is negligible. Since top or bottom product composition is of primary importance, and feedforward control does not have much effect on the product quality, there is hardly any justification for the use of combined feedforward-feedback control of the liquid temperature (or composi-

tion) on an intermediate tray. On the other hand, the addition of feedforward control to an existing feedback control loop of top or bottom product composition usually improves the control performance of the column as shown by Tables 6.4-6, 6.4-7, 6.4-13, 6.4-14, 6.4-19, 6.4-20, 6.4-25 and 6.4-26.

(viii) Although the selection of the overall performance index I.S.E. was arbitrary, it was found that the I.S.E. criterion generally gave results consistent with conventional concepts of "good control" as the control response is rapid, has minimum overshoot and small offset. Also, it was found that for control systems for which the column is inherently stable, it is difficult to determine the optimum controller settings exactly, since the I.S.E. value of the controlled variable is very small. However, it does not present any problem since settings near the optimum result in control which is nearly as satisfactory as that resulting when the exact values are used.

6.6-2 Discussion of Different Methods of Selecting the "Optimum" Control Tray Location

It can be seen from the results of section 6.5 that the selection of optimum control tray based on the simulation results did not agree very well with the selection of control tray using the methods suggested by Bertrand and Jones (14) and Uitti (15). This is understandable since with the methods of Bertrand and Jones and Uitti, the main concern is to determine the locations of the trays away from the ends of the column, where a large error signal to the controller is possible without sacrificing too much on product quality. With both

of these methods, no attention has been paid to the control performance of the column from either a dynamic or a steady-state standpoint. A constant liquid temperature (or composition) at one of these trays does not mean a constant product composition, as shown by the simulation results, and any offset present in the overhead or bottom product composition would be weighted heavily in the calculations of the performance index I.S.E. Meanwhile, in the simulation results, no allowance was made for possible inability of the temperature (or composition) transmitter to detect small variations in the controlled variable.

The choice of optimum control tray location using Rosenbrock's method (64) seems to agree with the selection based on the simulation results of the University of Delaware distillation column. It is possible that any agreement on the choice of the control tray by Rosenbrock's method and simulation results is purely by coincidence, since the principal purpose of the Rosenbrock method is to select the trays which will tend to bring the column as fast as possible toward some steady-state but this method does not ensure that this steady-state is the one desired.

Since the performance index I.S.E. of top or bottom product composition increases with the time if an offset is present in the product compositions, if the I.S.E. is evaluated over a long period, no doubt, the offset would be a predominant factor and in the end, the selection of the optimum control tray based on the minimum I.S.E. would be the same as the selection based on the minimum offset in product

compositions. Although the Wood method of selecting the control tray did not consider the control problem from a dynamic standpoint, the selection of control tray by this method will often give results that satisfy the control problem from both dynamic and steady-state considerations. Indeed, results from both distillation columns under investigation revealed that if reflux flow is used as the manipulative variable, the tray which gives the minimum steady-state error in the top product composition is close to the top of the column, therefore, in general the hydraulic lag in the control loop would be minimum. With steam flow as the manipulative variable, since the vapor flow is transmitted through the column very rapidly, steady-state error is the main factor in deciding upon the "optimum" control tray location.

In any event, the Wood method of tray-to-tray calculations is very helpful as it provides a convenient approach to calculate with reasonably high precision the steady-state offsets. These offsets, in general, can not be predicted accurately by a linear model. The non-linear behavior of the distillation column can be seen by examining Figures 6.5-4 through 6.5-7. It is apparent that the steady-state error of top or bottom product composition for a given change in feed flow rate does not have a fixed value, but varies according to the initial steady-state conditions. For instance Figure 6.5-7 shows that if the initial steady-state value of bottom composition is 0.6 per cent methanol, a decrease in feed flow rate from 50 per cent to 40 per cent results in an increase of 0.28 per cent in bottom product composition

if the liquid temperature on tray 1 is kept constant by manipulation of the steam flow. However, it can be seen that if the initial steady-state value of bottom product composition is only 0.4 per cent methanol, and the liquid temperature on tray 1 is kept constant, no offset in bottom composition would result.

CHAPTER VII

EXPERIMENTAL RESULTS

7.1 Introduction

The experimental work was carried out on the University of Alberta distillation column. This column is interfaced with an IBM 1800 digital computer. The availability of a process control computer permits not only the substitution of the conventional equipment by using direct digital control (DDC) but it also allows the processing of a large amount of data acquisition and logging.

A series of experimental tests were conducted to determine the usefulness of empirical models in predicting the control response of the distillation column and to compare the actual performance of the column at different proposed locations of the sensor.

7.2 Description of Experimental Equipment

The pilot-scale distillation column used in this study contains eight plates and is nine inches in diameter. The glass column is equipped with a total condenser and a basket type reboiler. The trays were of the bubble cap type and each tray is fitted with four 2 1/4 x 1 7/8-inch diameter bubble caps, 1 1/2-inch diameter inlet and outlet weirs and an 1-inch diameter downcomer. The condenser consists of a bundle of stainless steel tubes in a nine-inch diameter by three-foot long glass shell, and the reboiler which is of 7-inch nominal

diameter contained thirty eight, one-half-inch diameter by twenty four-inch long heating tubes.

Feed of a predetermined composition drawn from either one of two storage feed tanks, each of 200 gallon capacity, was fed to the column at tray 4 (counted from the bottom upwards) and products were combined and returned to the same tank, hence an unlimited number of experimental runs could be performed without shutting down the column. Feed can also be introduced at tray 5, and if top and bottom products are desired, they can be returned to two separate glass lined tanks. Steam preheaters installed on the feed and reflux lines were standard, single pass, shell and tube heat exchangers.

Two different instrumentation systems are currently available for control of this distillation column: conventional analog and computer control using the IBM 1800 digital computer. Presently, the control of condenser and reboiler liquid levels, feed and reflux temperatures, and pressure in the condenser is only possible using conventional analog controllers. The tower differential pressure was measured but not used for control of the steam flow rate entering the column. The system is designed so that if only feedback control of top product composition is desired, the column can be operated with or without the computer. The control of the liquid temperature on an intermediate tray or bottom product composition is implemented by means of the computer.

The overhead product composition was continuously monitored

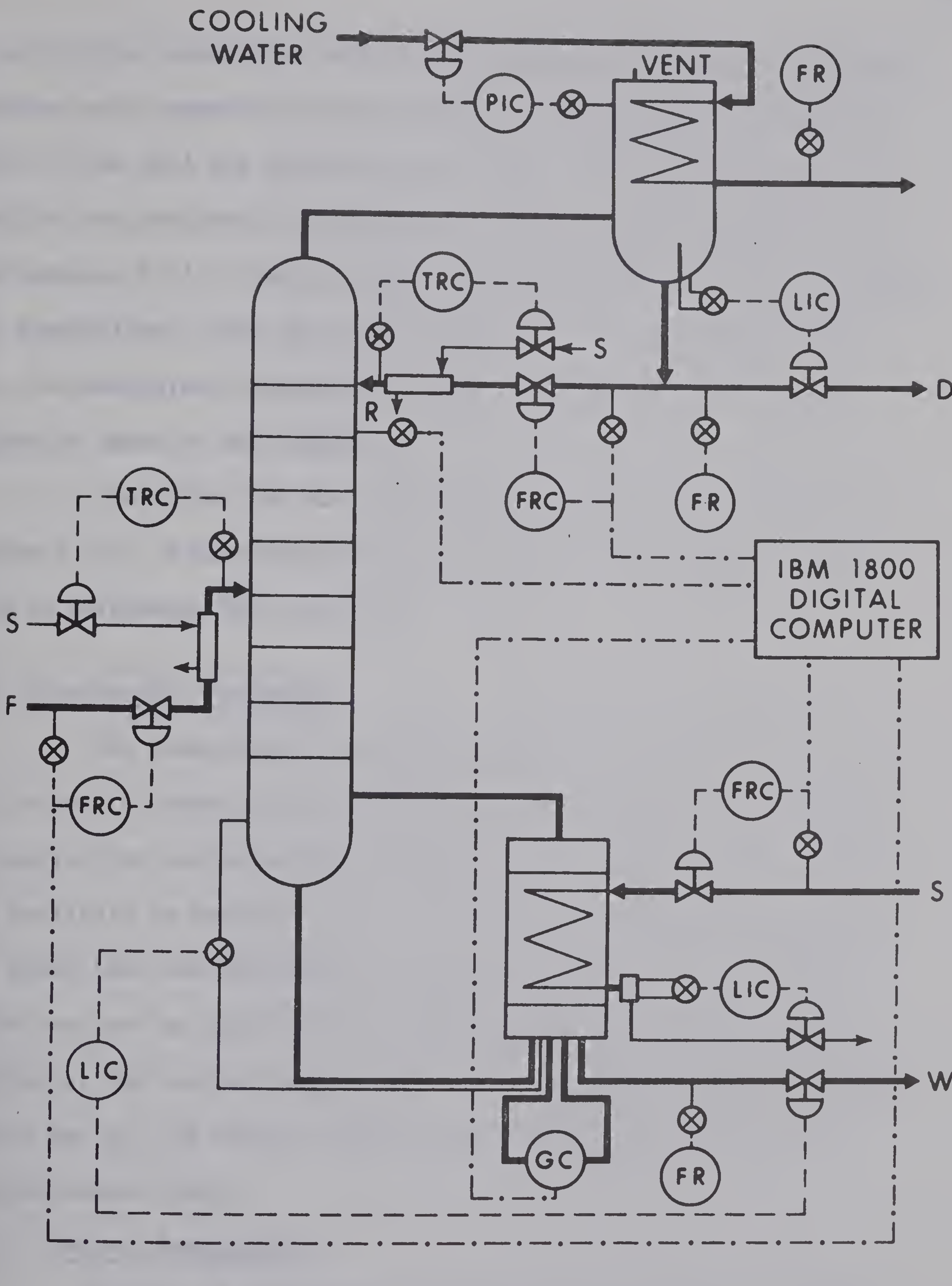


Figure 7.2-1 Schematic Diagram of the Distillation Column
and Its Associated Instrumentation

by an in-line capacitance cell and the measure of change in dielectric constant with composition was tranduced to the computer. Design details of the cell are given by Svrcek (73). The bottom product composition was analyzed by a process gas chromatograph interfaced with the computer (11). Iron-constantan thermocouples were used to measure all temperatures. All the analog signals from the sensing devices i.e. thermocouples, flowmeters, pressure transducer, etc....were logged by means of the computer.

The column and its associated instrumentation is shown in Figure 7.2-1. A more detailed description of the equipment is available in References (51) and (73).

7.3 Experimental Procedure

The experimental procedure consisted initially of bringing the column to steady-state and starting up the gas chromatograph used to analyze the bottom product composition. These start-up procedures are available in Reference (51). The following description outlines the steps that are required to initiate and complete a fully documented run on the distillation column, assuming that the column is running at the desired steady-state with the desired control configuration and all the direct digital control (DDC) loops are in the operable-manual mode.

7.3.1 Pre-run Preparation

Samples of both feed and bottom product streams are taken and their compositions are measured. These measurements are required

to establish both mass and energy balances. The DDC loop monitoring the liquid temperature on an intermediate tray should have the desired controller constants and its set point should be set at the same value as its current measurement. This primary temperature control loop would then be switched to operable automatic-mode.

7.3.2 <u>Initial Steady-State Documentation</u>

Steady-state material and energy balances around the distillation column were made for each run by queuing the process program DASS. All the process variables which have been interfaced with the IBM 1800 computer are recorded at every scan time (for example 10 seconds) for a certain number of times (for example 10 times if the steady-state calculations were made over 100 seconds), then averaged and the results printed out on the IBM 1132 line printer. The number of sampling points (i.e. 10) and the scan time (i.e. 10) are specified and can be modified by the user through the teletype. A typical output is shown in Appendix D.

7.3.3 <u>Experimental Test Documentation</u>

After the steady-state material and energy balances were computed and agree within about five per cent; initialization of data acquisition of various process variables can be started by queuing the process program ONOFF from the teletype. This program has two main functions: Buffering data to disk and monitoring the gas chromatograph.

(i) Buffering data to disk. The ONOFF program ensures that all

the necessary DDC control, data accumulation loops and ring buffers are operable by entering the following options through the teletype:

- Option 1: to make all the DDC control and data accumulation loops operable.

- Option 3: to make all the ring buffers operable.

The DDC file counter should be initialized by using option 5.

(ii) Monitoring the gas chromatograph. - Option 8 of ONOFF program permits the user to sample, analyze and print out the bottom or feed composition. Sub-option 0 is used if bottom product composition is to be measured and sub-option 1 is used if feed composition is desired. Once initialized, this program is automatically activated every 2.5 minutes if bottom product composition is desired and every 3.0 minutes if feed composition is desired.

After ONOFF is queued, approximately 10 to 15 minutes is allowed for initial steady-state data accumulation before the disturbance is entered. The feed flow disturbance was introduced into the distillation column by changing the output of the feed flow rate DDC control loop by means of the teletype.

7.3.4 Test Termination

When the test was completed, after approximately two to two and half hours of operation, a print out of the final steady-state documentation was obtained by queuing the DASS process program. When the documentation was complete, the ONOFF program was then queued.

Option 4, once entered, stopped the buffering of data to disk, option 2 made all the control and data acquisition non-operable and finally option 9 terminated sampling and analysis of the bottom product (or feed) composition.

7.3.5 Post-test Documentation

The transient data buffered to disk must be recovered before the DDC file counter is reinitialized for another experimental run. This is done by using the nonprocess program GTDAT. This program prints out the data from disk on the IBM 1132 line printer and punches the data onto cards for future processing.

The listings for all these programs appear in Appendix D.

7.4 Results

The control behavior of the distillation column under feedback control of the liquid temperature on an intermediate tray was studied for increases and decreases in feed flow rate. An increase in feed flow rate is a step change from 50 per cent to 70 per cent on the feed flow recording chart (which corresponds to a change from 2.47 lb./min. to 2.90 lb./min.) while a decrease in feed flow rate refers to a step change from 50 to 30 per cent on the chart which is equivalent to a change from 2.47 lb./min. to 1.93 lb./min.

As an experimental investigation of temperature control of the liquid on every single individual tray would prove too time consuming, only temperature control of the liquid on some selected trays was studied. To evaluate the control scheme using reflux flow as the

manipulative variable, trays 7 and 8 were successively chosen as the control tray. The selection of tray 8 is desired because simulation results revealed that it is the optimum tray to control top product composition. Tray 7 was chosen to study the effects of locating the control tray down the column to get a larger error signal for the temperature controller.

To evaluate the control scheme using steam flow as the manipulative variable, the control performance of the column was investigated when the sensor was successively located on trays 6 and 1; Tray 6 was chosen as one of the control trays for the experimental work since simulation results showed that it is the best tray to use for control of the overhead composition. Tray 1 was selected to study the effect on the control performance of locating the sensor close to the control valve.

The temperature control loop was implemented by using the DDC package available on the IBM 1800. A sampling time of two seconds was chosen in order to minimize the effect of sampling time upon the control behavior of the column. The following two cases were investigated:

(i) Feedback control of the liquid temperature on an intermediate tray using a proportional plus integral control algorithm.

Objective: Minimize the I.S.E. value for the liquid temperature on the control tray.

Optimum controller settings: Table 7.4-1.

Typical column responses: Figures 7.4-1 to 7.4-8.

(ii) Feedback control of the liquid temperature on an intermediate tray using a proportional control algorithm.

Objective: Minimize the I.S.E. value for the overhead composition.

Optimum controller settings: Table 7.4-2.

Typical column responses: Figures 7.4-9 to 7.4-16.

The optimum controller settings given in Tables 7.4-1 and 7.4-2 were determined empirically by varying different loop words corresponding to the proportional controller gain and the integral time in the DDC loop record. The control action of the proportional plus integral DDC controllers can be expressed as

$$m(t) = K_p\, e(t) + K_p \times K_i\, \Sigma\, e(t) + m_0 \qquad (7.4\text{-}1a)$$

or

$$m(t) = K_p\, e(t) + K_p \times \frac{\Delta t}{\tau_I}\, \Sigma\, e(t) + m_0 \qquad (7.4\text{-}1b)$$

where $m(t)$ is the output signal of DDC algorithm at any time, m_0 is the output signal of DDC algorithm at previous calculation and Δt is the DDC sampling time.

Although the I.S.E. index performance was calculated during each experimental run, it was not used as the sole criterion in determining the optimum controller constants due to the presence of noise in the process. In most cases, the satisfactory empirical controller

Table 7.4-1

Optimum Controller Constants for Temperature Control Loops

(Objective: constant liquid temperature on the intermediate control tray)

Manipulative Variable	Control Tray	Magnitude of Disturbance (CHART PER CENT)**	K_p*	τ_1* (sec.)
Reflux Flow	8	+ 20%	224.0	128.0
	8	- 20%	224.0	128.0
	7	+ 20%	250.0	160.0
	7	- 20%	224.0	160.0
Steam Flow	6	+ 20%	45.0	270.0
	6	- 20%	64.0	270.0
	1	+ 20%	24.0	120.0
	1	- 20%	24.0	120.0

*DDC values as given by equation (7.4-1a) or (7.4-1b).

**+20% is equivalent to a step change from 2.47 lb./min. to 2.90 lb./min.
-20% is equivalent to a step change from 2.47 lb./min. to 1.93 lb./min.

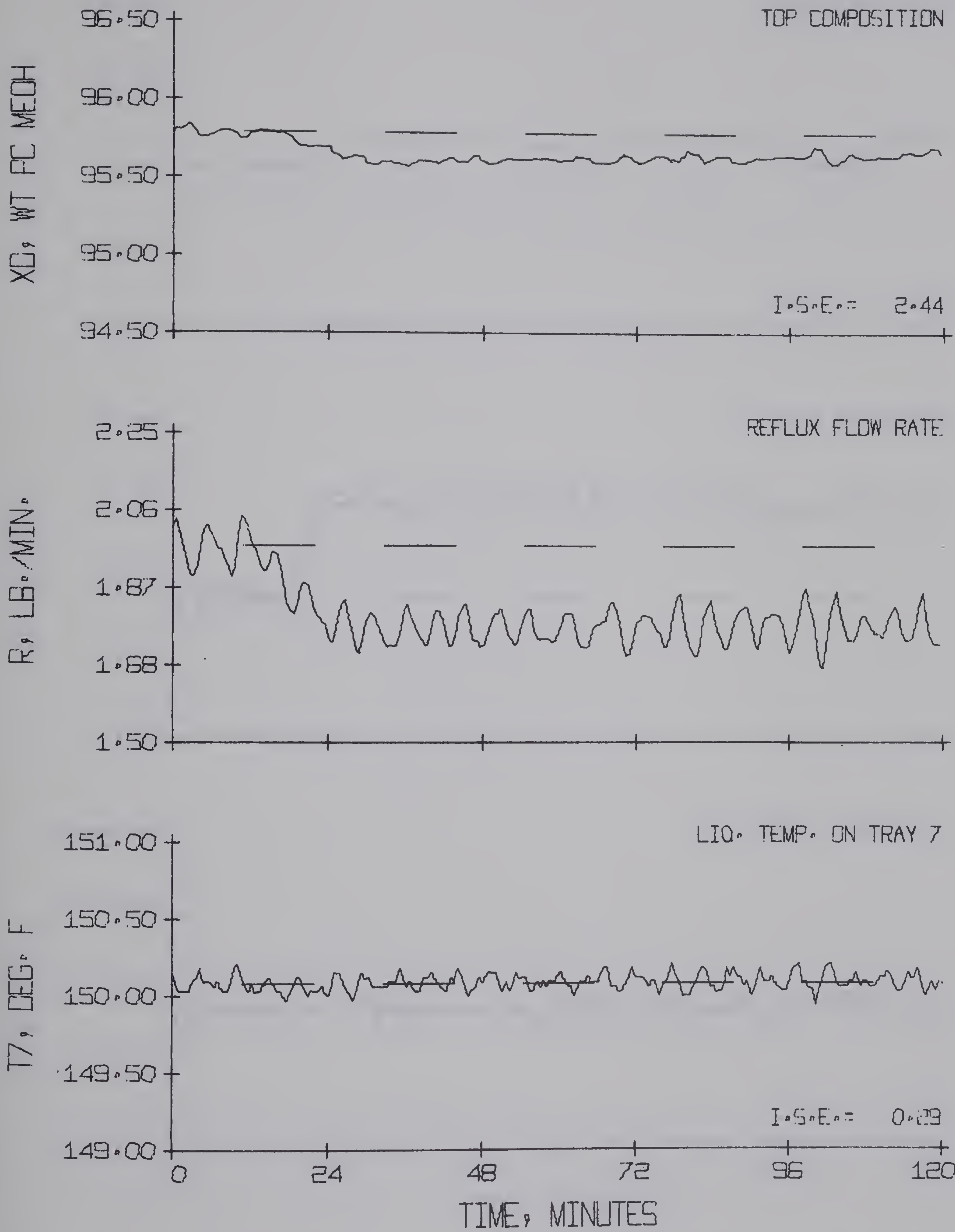


Figure 7.4-1 Feedback Control of the Liquid Temperature on Tray 7 by Manipulation of Reflux Flow - PI Feedback Controller (50% - 70% step change in feed flow)

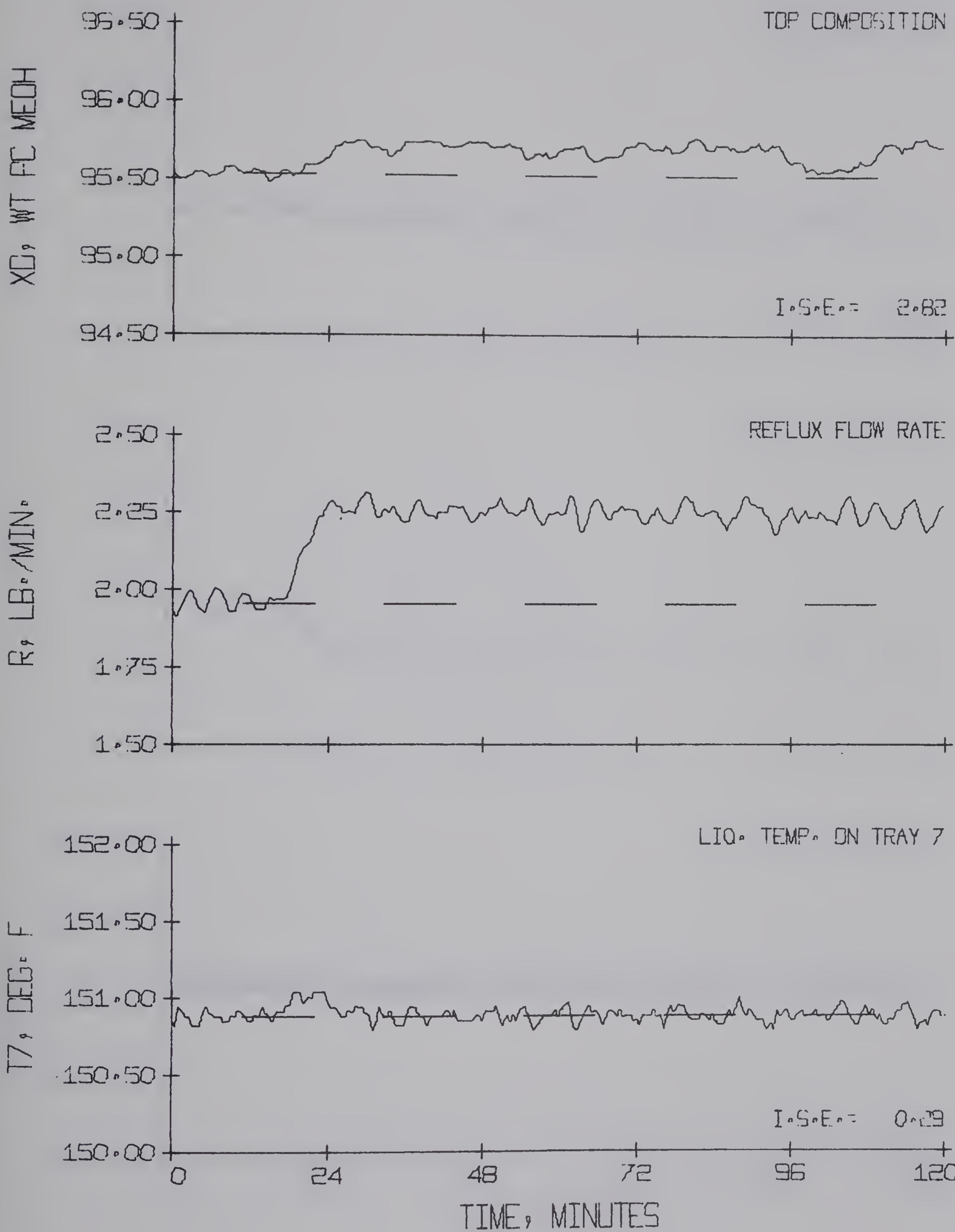
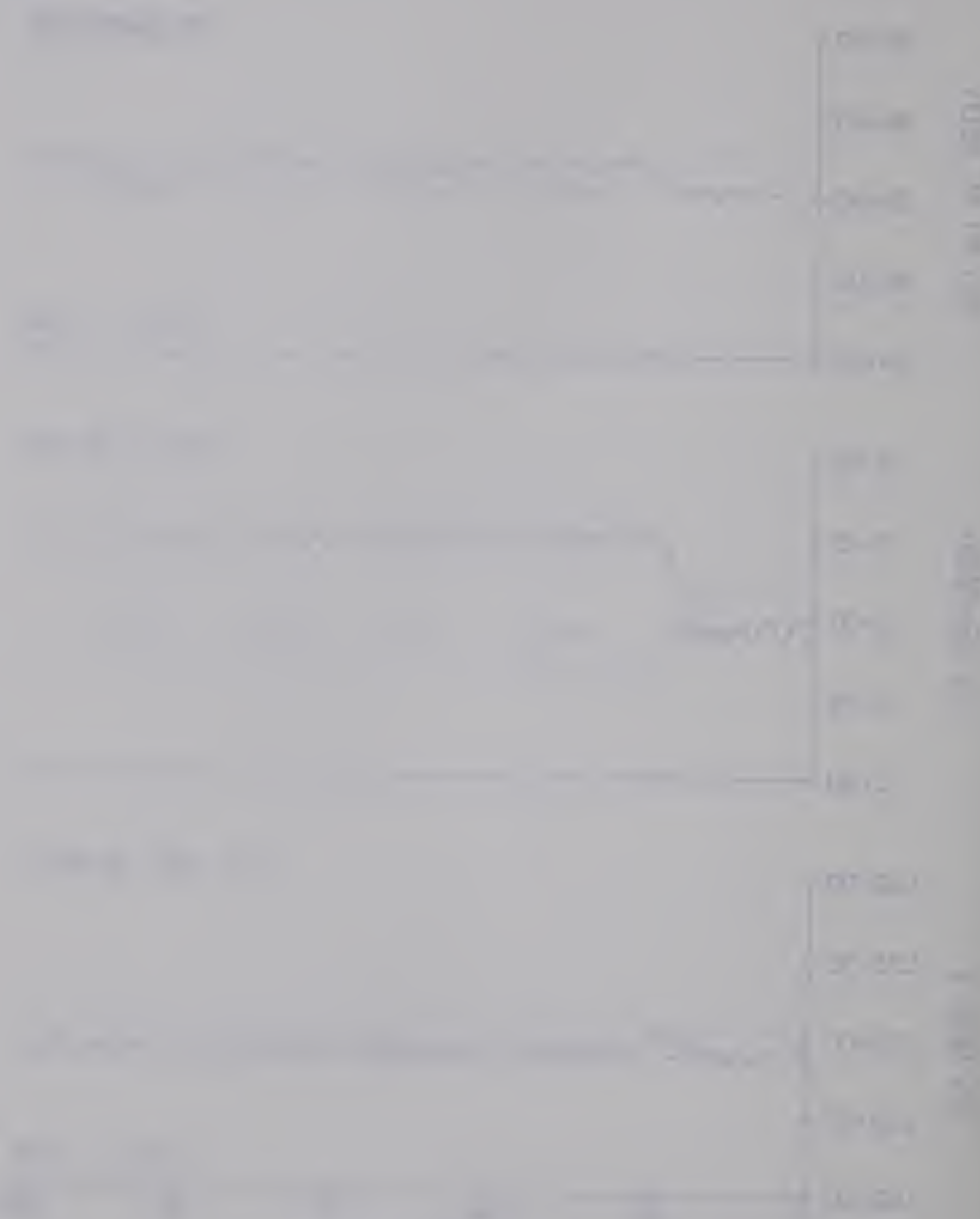


Figure 7.4-2 Feedback Control of the Liquid Temperature on Tray 7 by Manipulation of Reflux Flow - PI Feedback Controller (50% - 30% step change in feed flow)



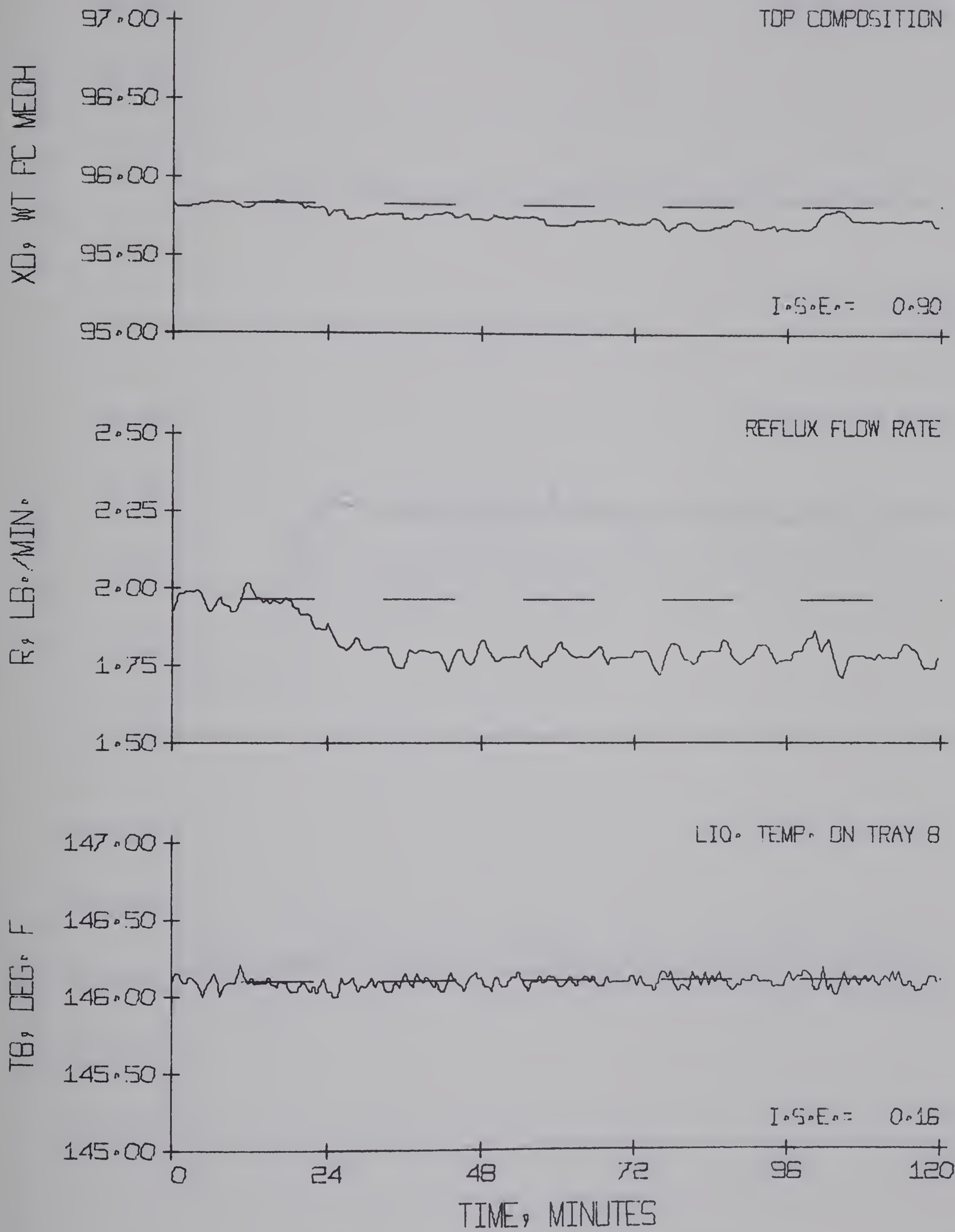


Figure 7.4-3 Feedback Control of the Liquid Temperature on Tray 8 by Manipulation of Reflux Flow - PI Feedback Controller (50% - 70% step change in feed flow)

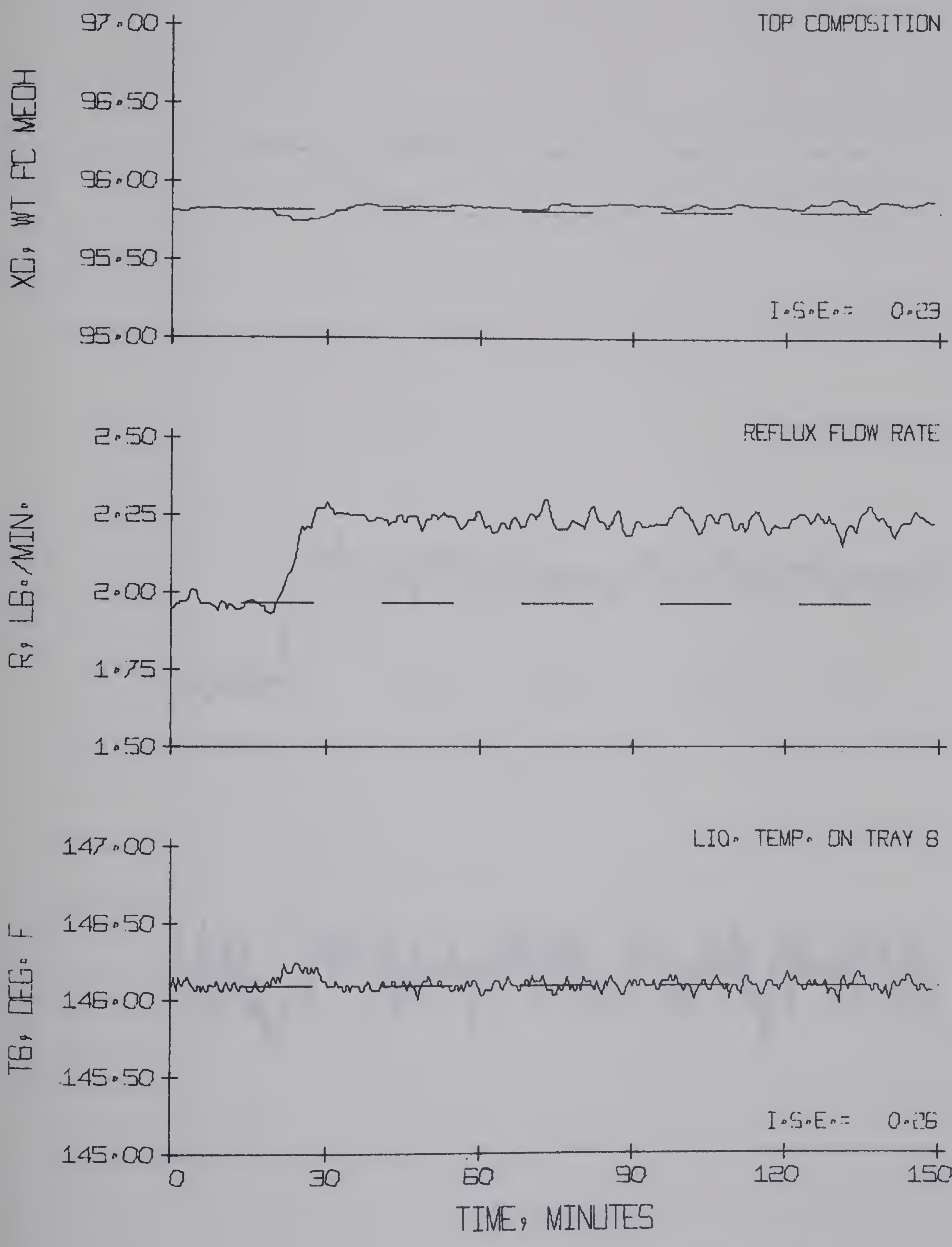


Figure 7.4-4 Feedback Control of the Liquid Temperature on Tray 8 by Manipulation of Reflux Flow - PI Feedback Controller (50% - 30% step change in feed flow)

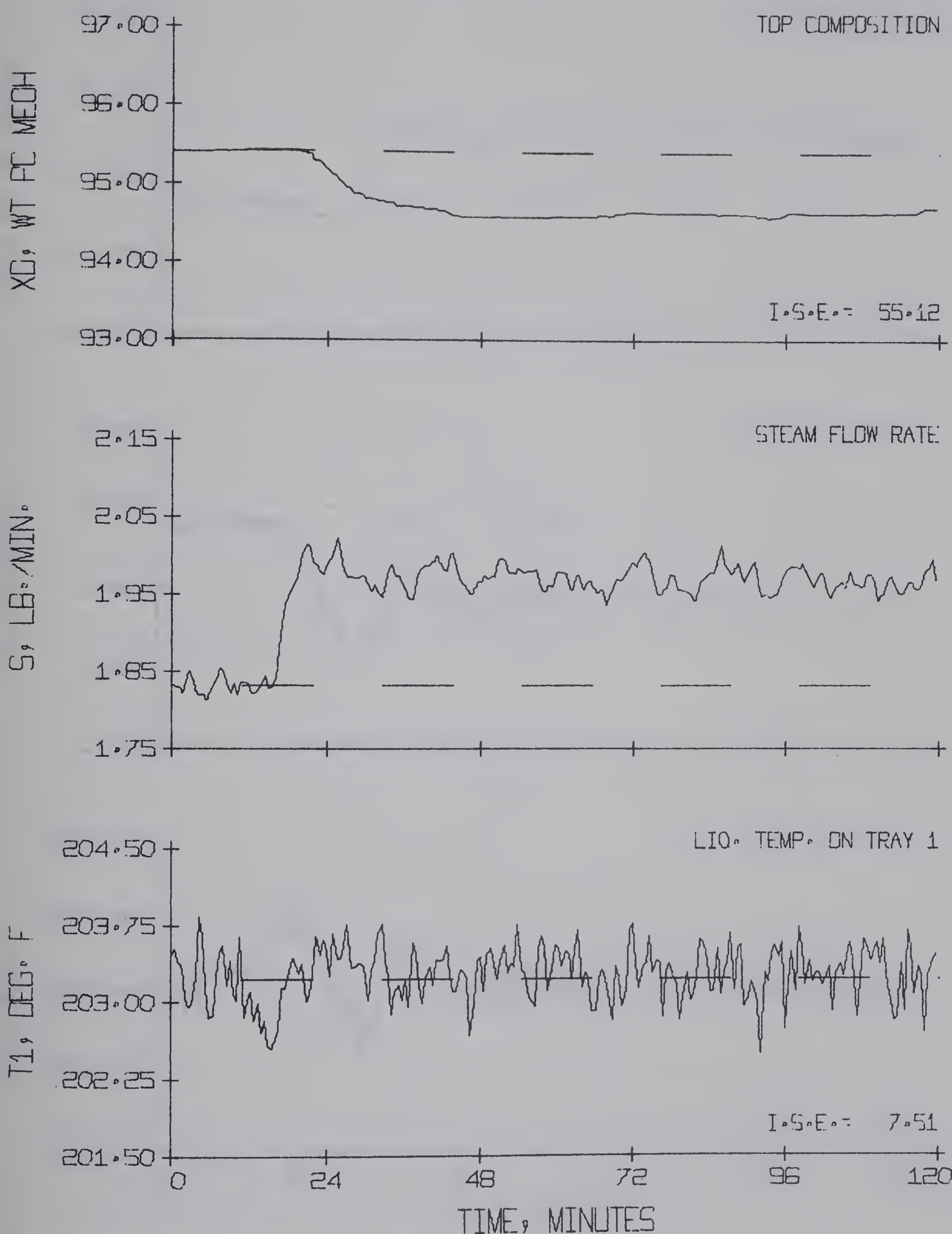


Figure 7.4-5 Feedback Control of the Liquid Temperature on Tray 1 by Manipulation of Steam Flow - PI Feedback Controller (50% - 70% step change in feed flow)

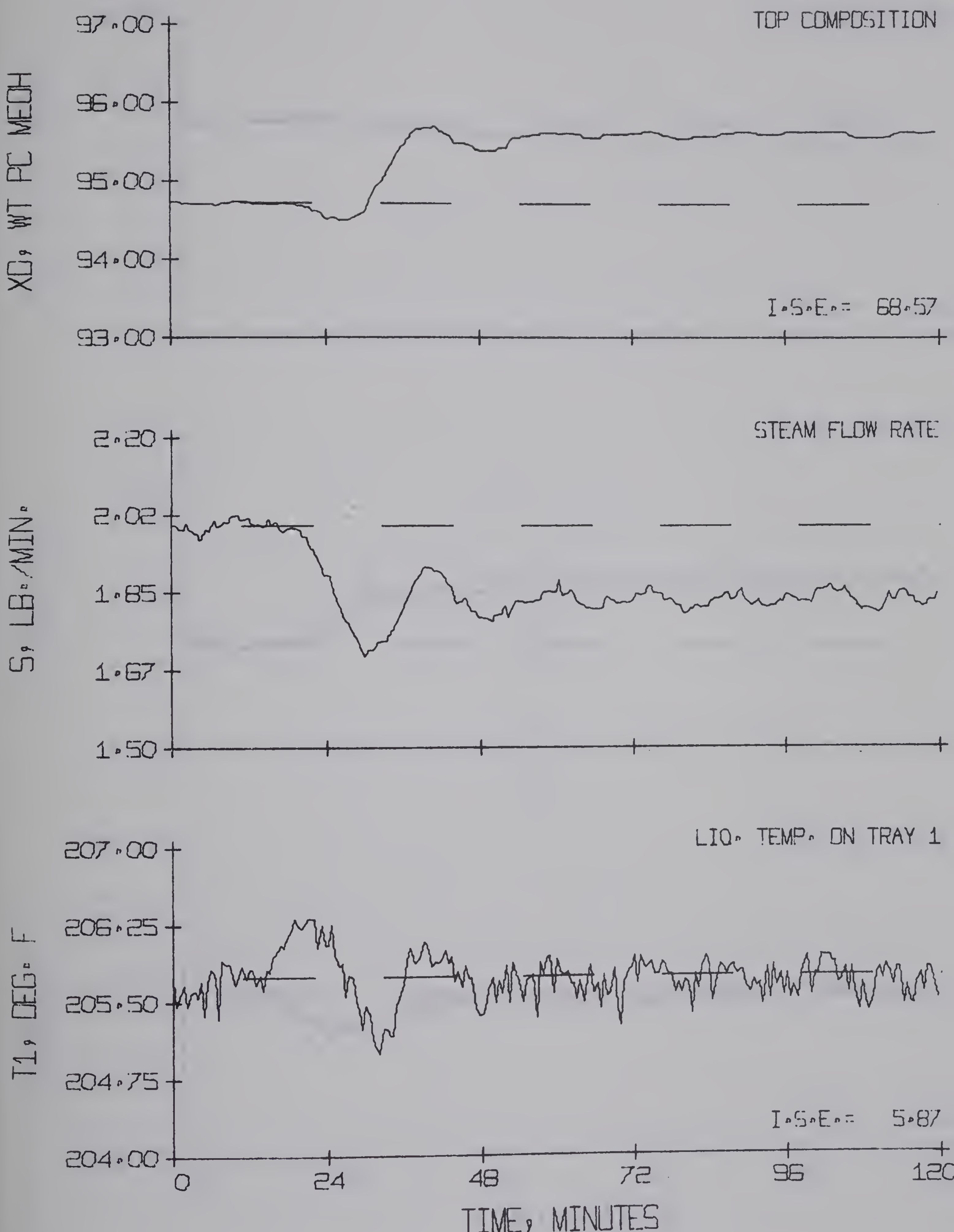


Figure 7.4-6 Feedback Control of the Liquid Temperature on Tray 1 by Manipulation of Steam Flow - PI Feedback Controller (50% - 30% step change in feed flow)

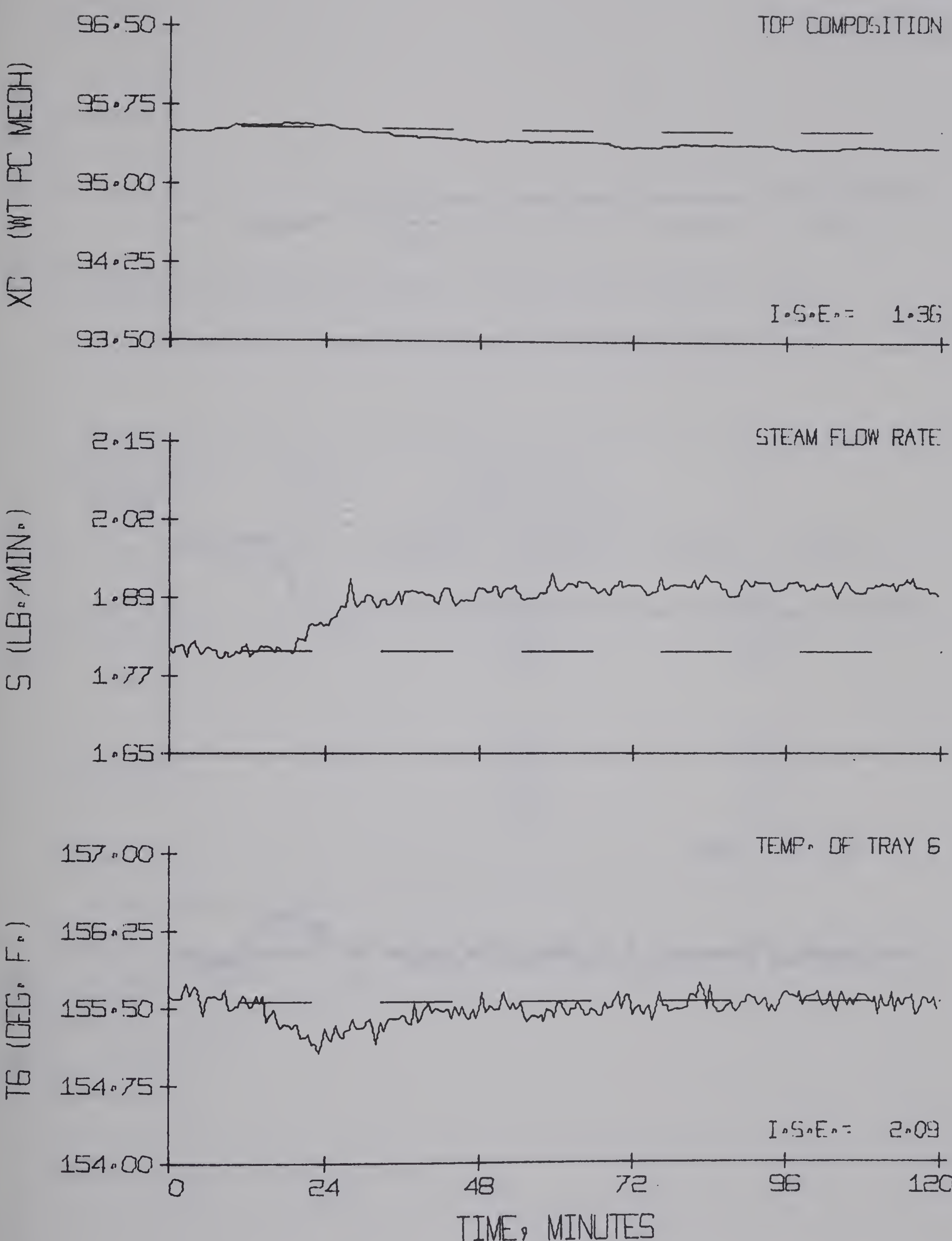


Figure 7.4-7 Feedback Control of the Liquid Temperature on Tray 6 by Manipulation of Steam Flow - PI Feedback Controller (50% - 70% step change in feed flow)

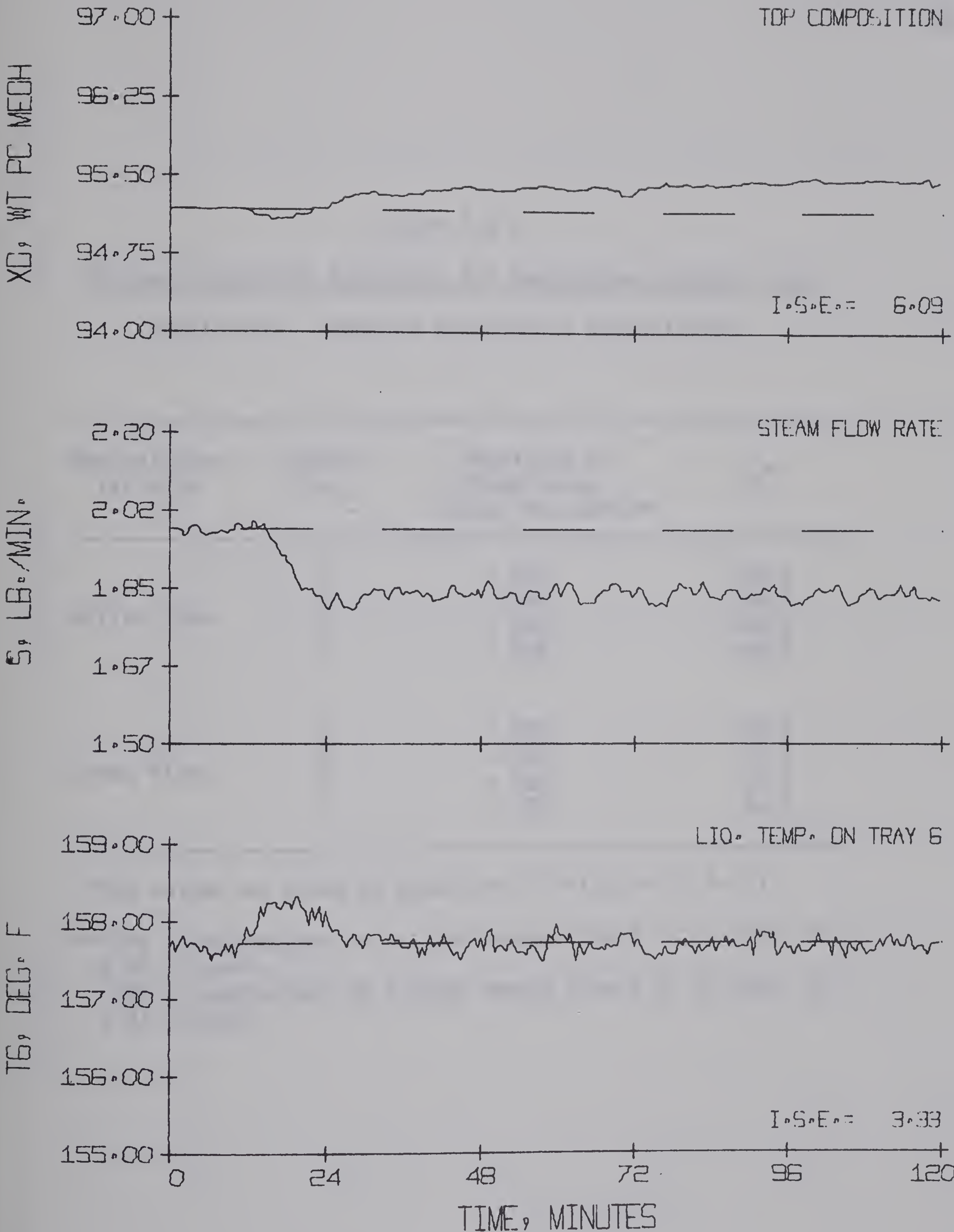


Figure 7.4-8 Feedback Control of the Liquid Temperature on Tray 6 by Manipulation of Steam Flow - PI Feedback Controller (50% - 30% step change in feed flow)

Table 7.4-2

Optimum Controller Constants for Temperature Control Loops

(Objective: constant top product composition)

Manipulative Variable	Control Tray	Magnitude of Disturbance (CHART PER CENT)**	K_p*
Reflux Flow	8	+ 20%	256.0
	8	- 20%	256.0
	7	+ 20%	190.0
	7	- 20%	208.0
Steam Flow	6	+ 20%	103.0
	6	- 20%	75.0
	1	+ 20%	10.5
	1	- 20%	63.0

*DDC values as given by equation (7.4-1a) or (7.4-1b).

**+20% is equivalent to a step change from 2.47 lb./min. to 2.90 lb./min.
-20% is equivalent to a step change from 2.47 lb./min. to 1.93 lb./min.

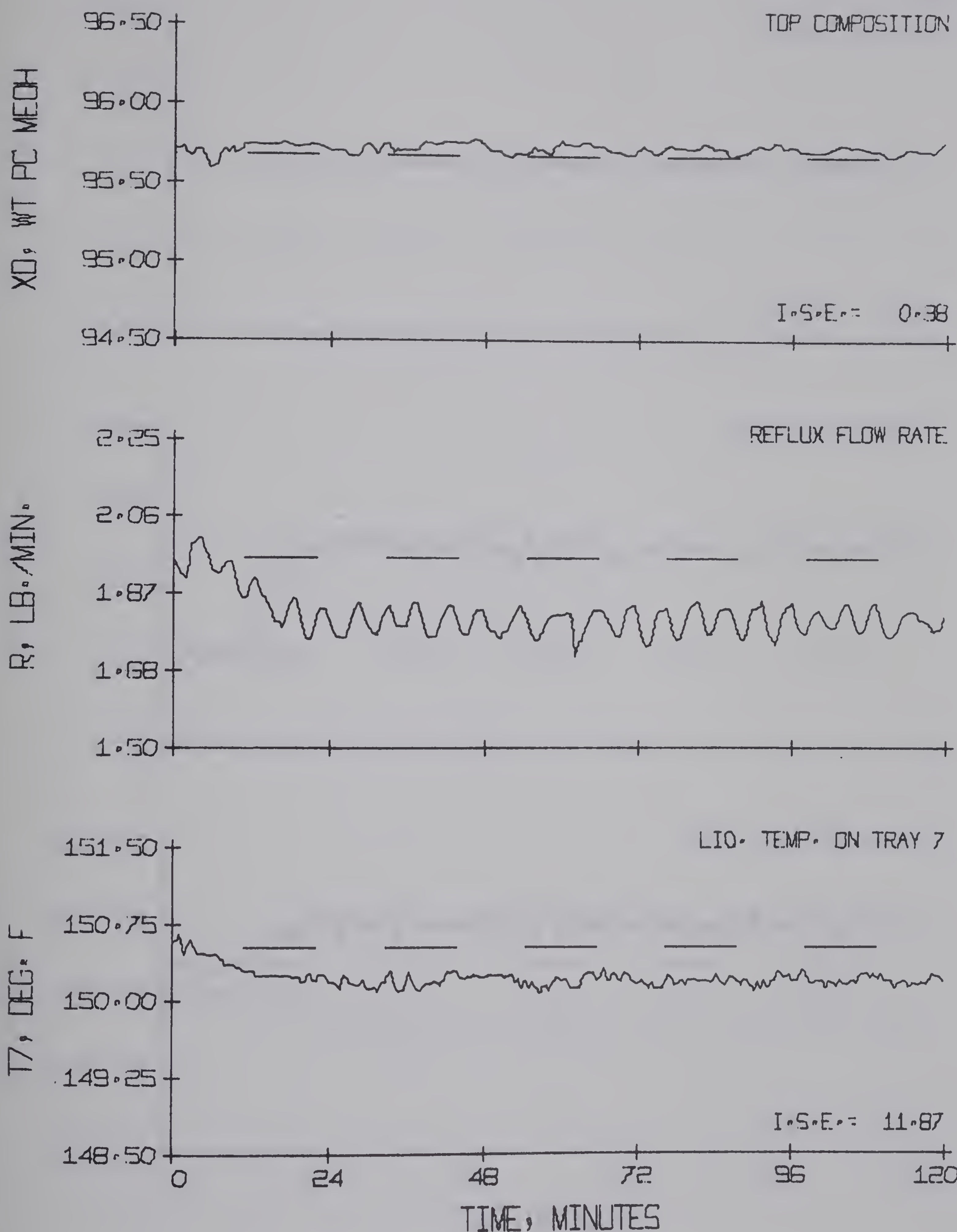


Figure 7.4-9 Feedback Control of the Liquid Temperature on Tray 7 by Manipulation of Reflux Flow - Proportional Feedback Controller (50% - 70% step change in feed flow)

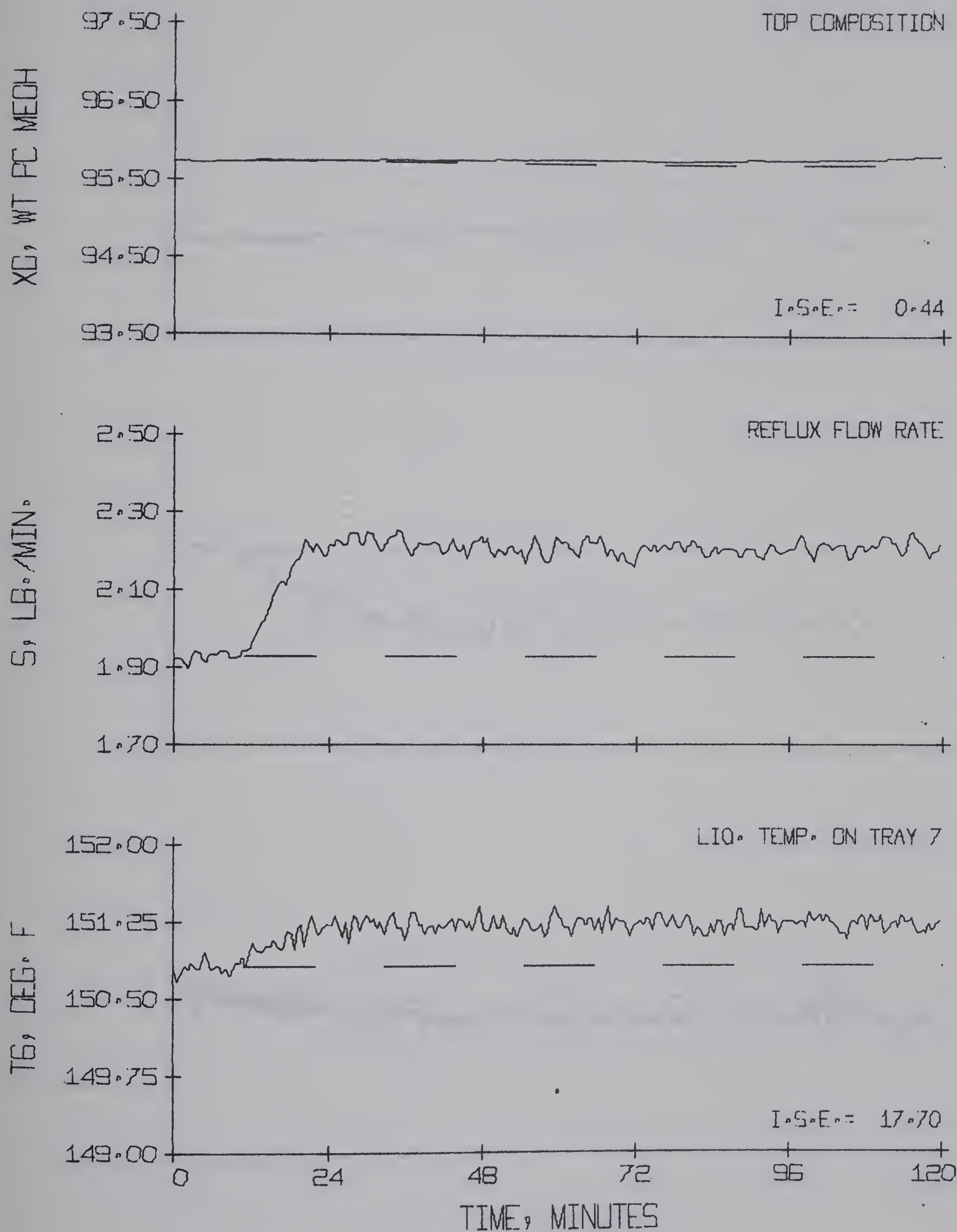


Figure 7.4-10 Feedback Control of the Liquid Temperature on Tray 7 by Manipulation of Reflux Flow - Proportional Feedback Controller (50% - 30% step change in feed flow)

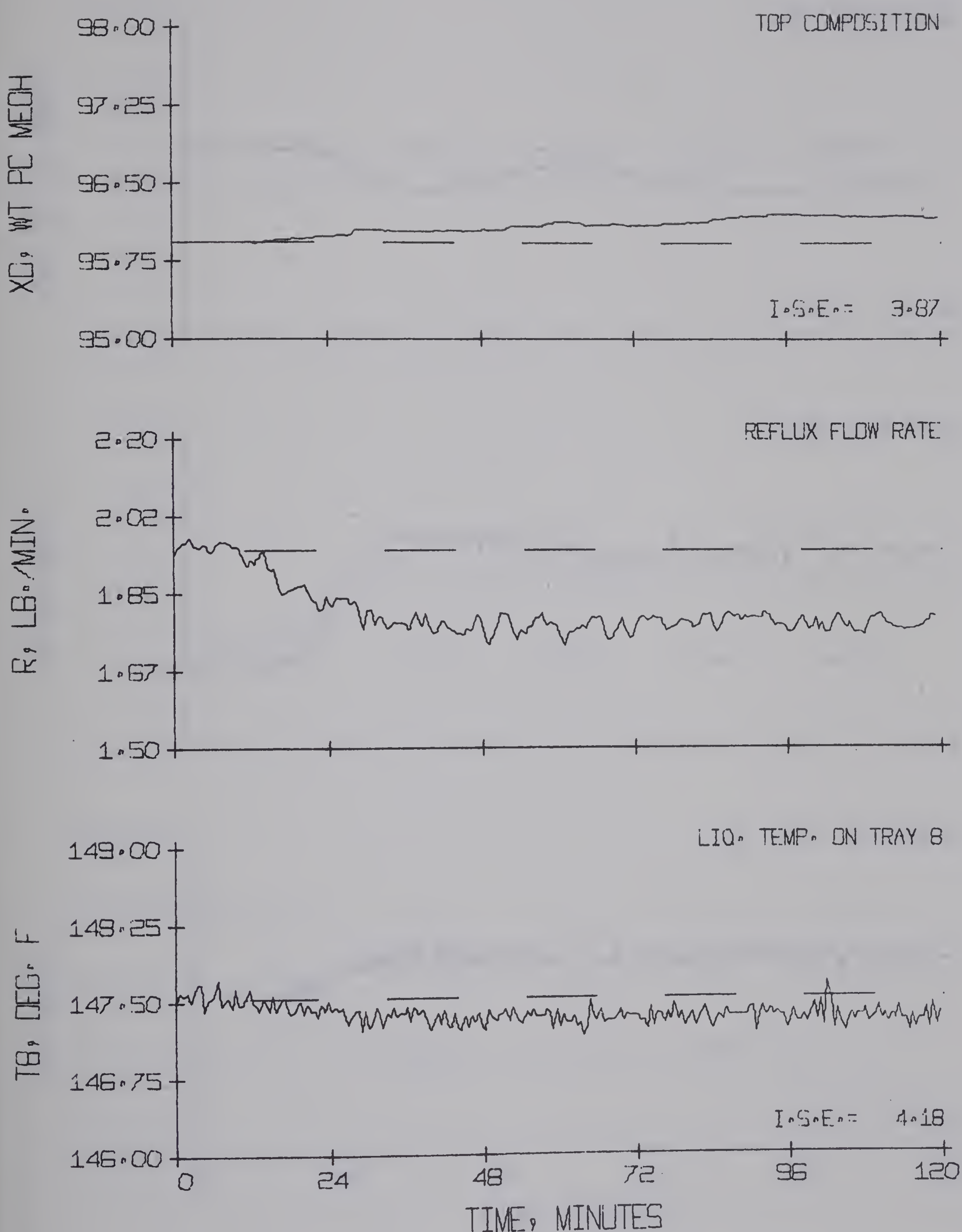


Figure 7.4-11 Feedback Control of the Liquid Temperature on Tray 8 by Manipulation of Reflux Flow - Proportional Feedback Controller (50% - 70% step change in feed flow)

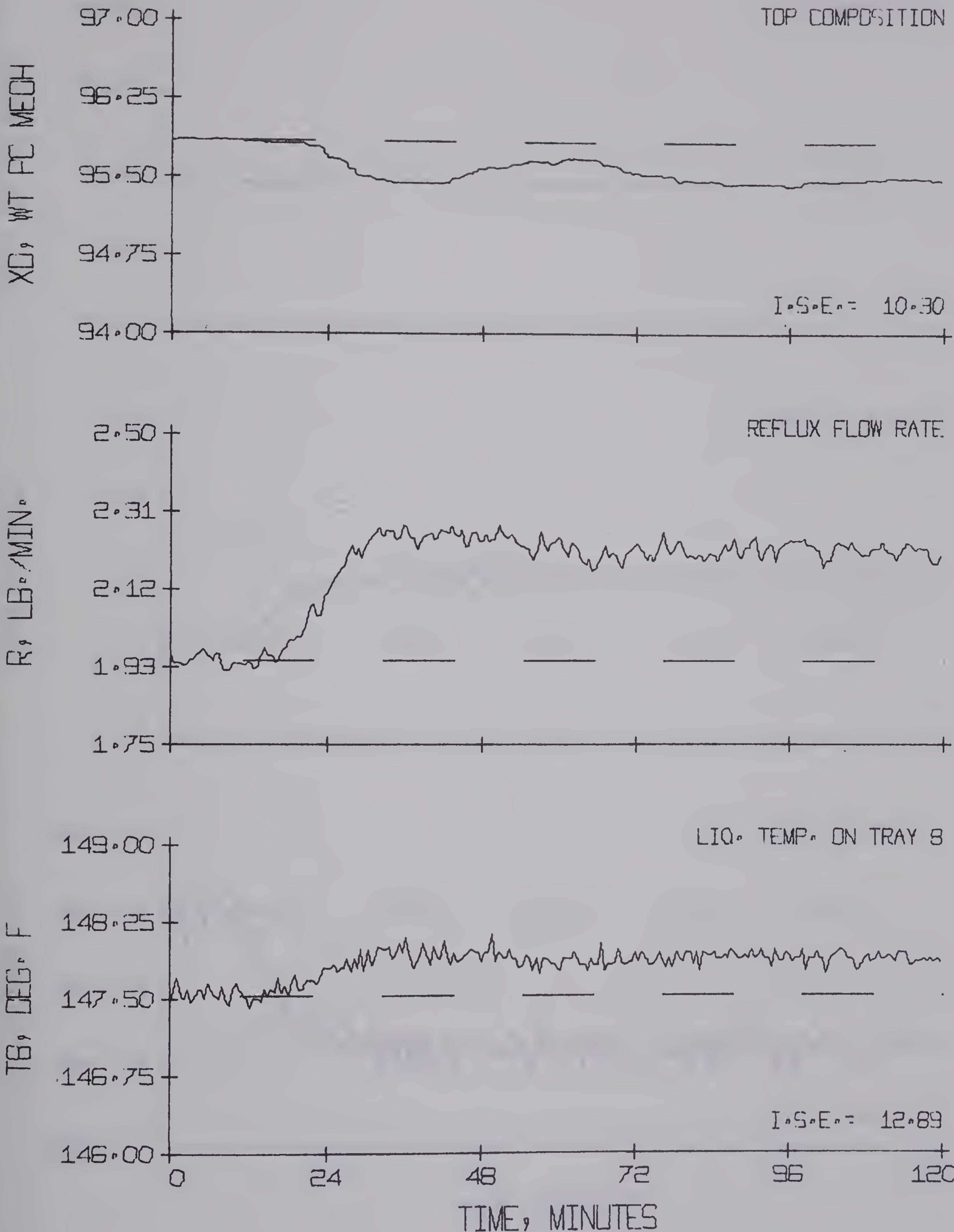


Figure 7.4-12 Feedback Control of the Liquid Temperature on Tray 8 by Manipulation of Reflux Flow - Proportional Feedback Controller (50% - 30% step change in feed flow)

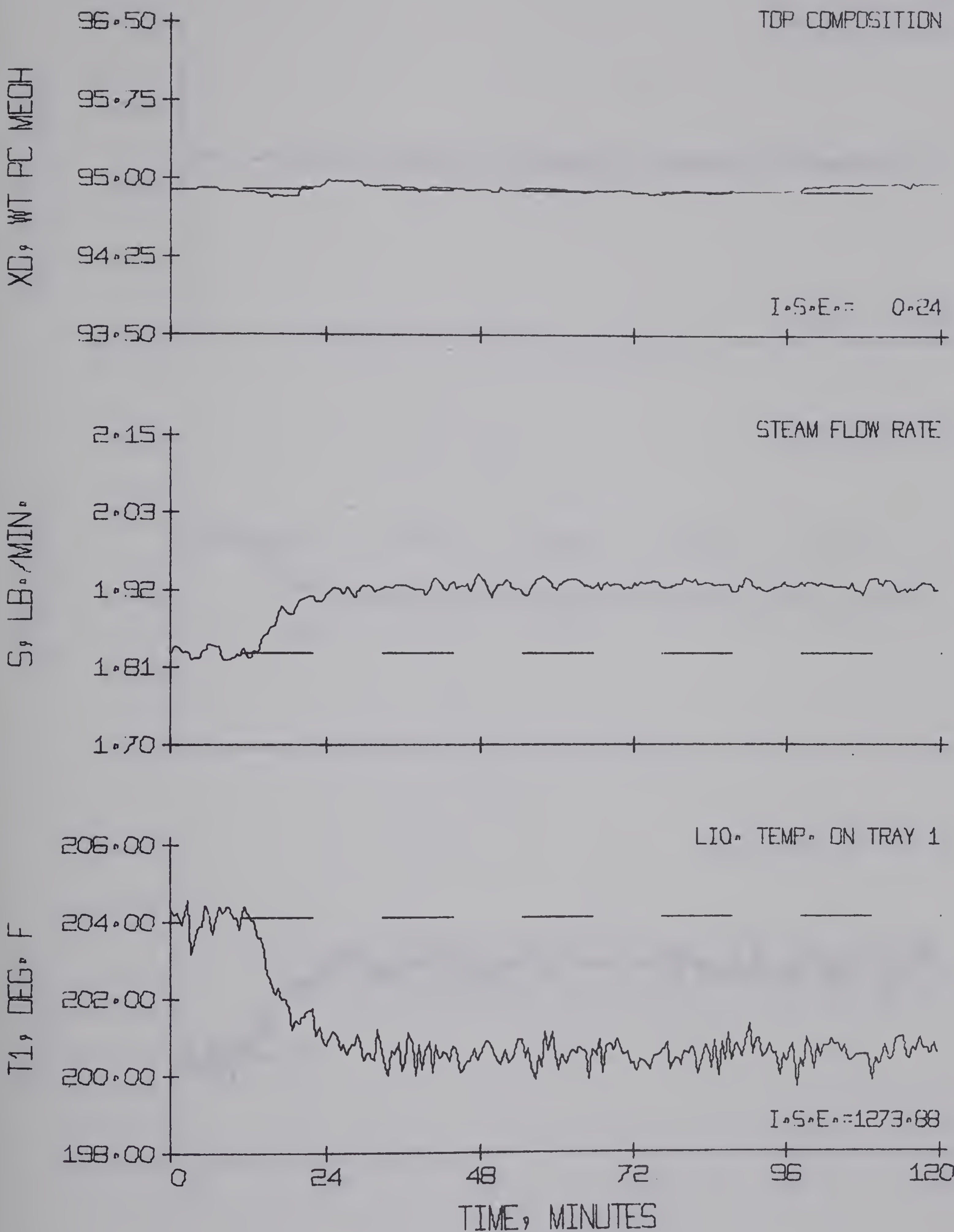


Figure 7.4-13 Feedback Control of the Liquid Temperature on Tray 1 by Manipulation of Steam Flow - Proportional Feedback Controller (50% - 70% step change in feed flow)

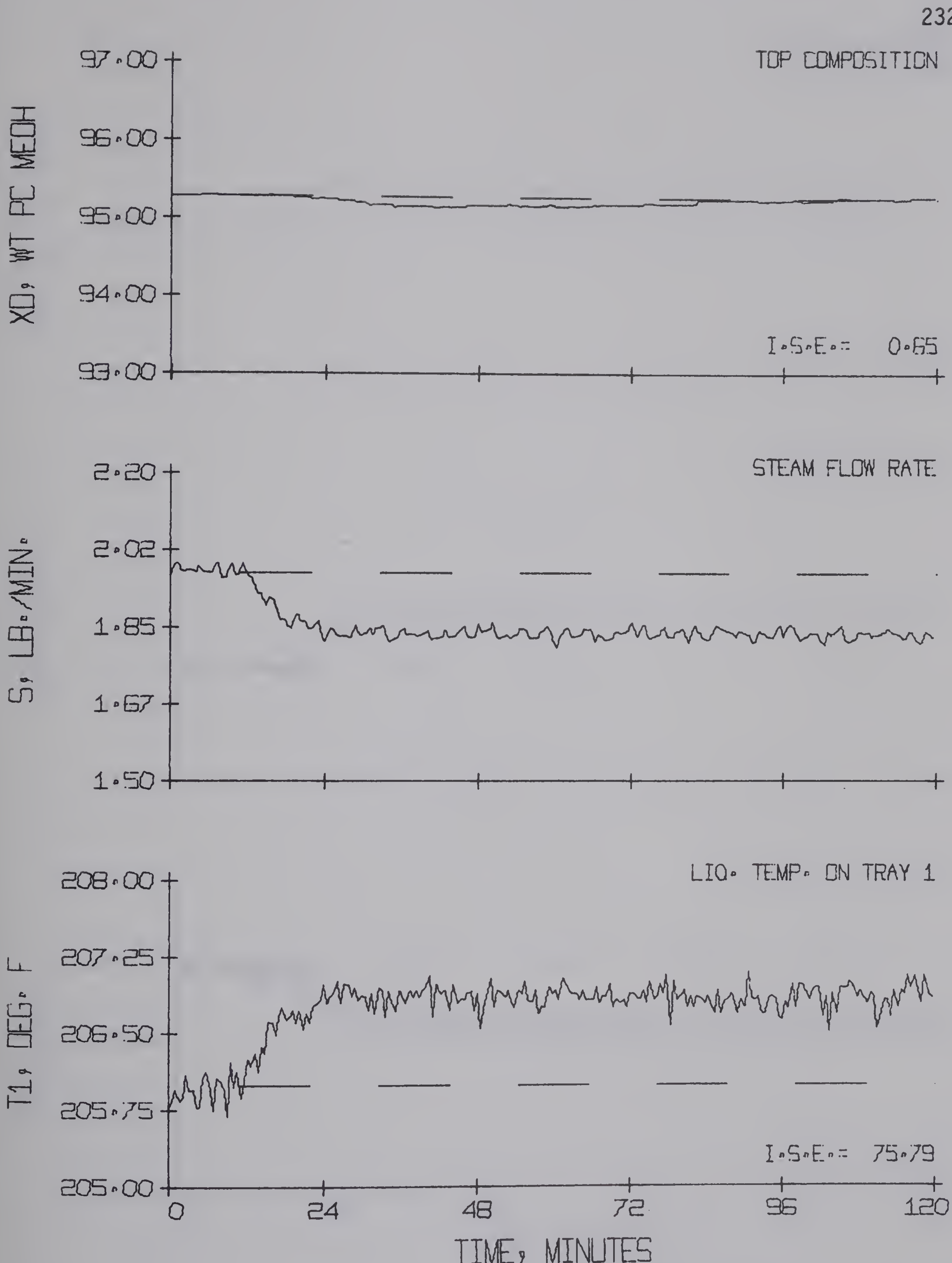


Figure 7.4-14 Feedback Control of the Liquid Temperature on Tray 1 by Manipulation of Steam Flow - Proportional Feedback Controller (50% - 30% step change in feed flow)

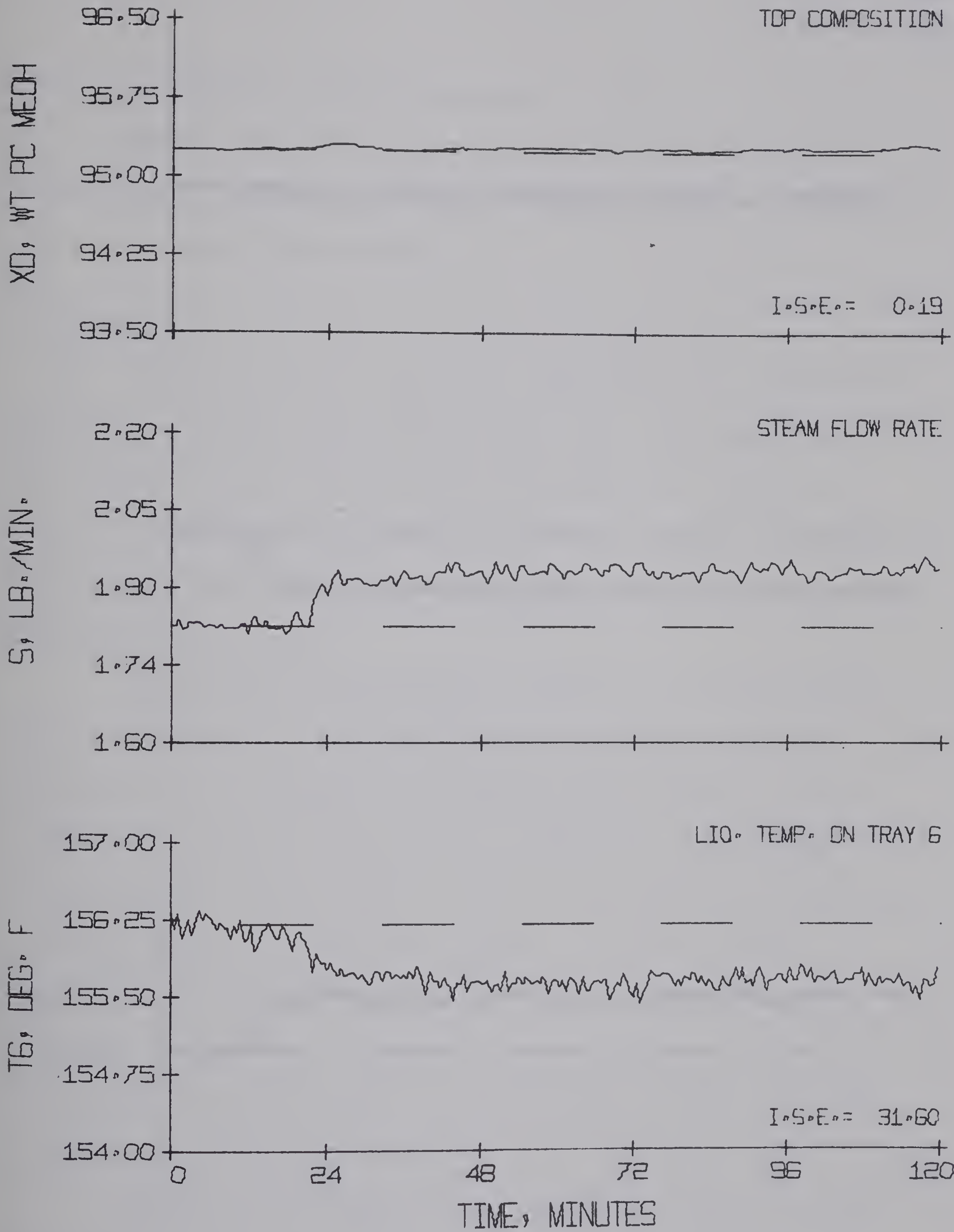


Figure 7.4-15 Feedback Control of the Liquid Temperature on Tray 6 by Manipulation of Steam Flow - Proportional Feedback Controller (50% - 70% step change in feed flow)

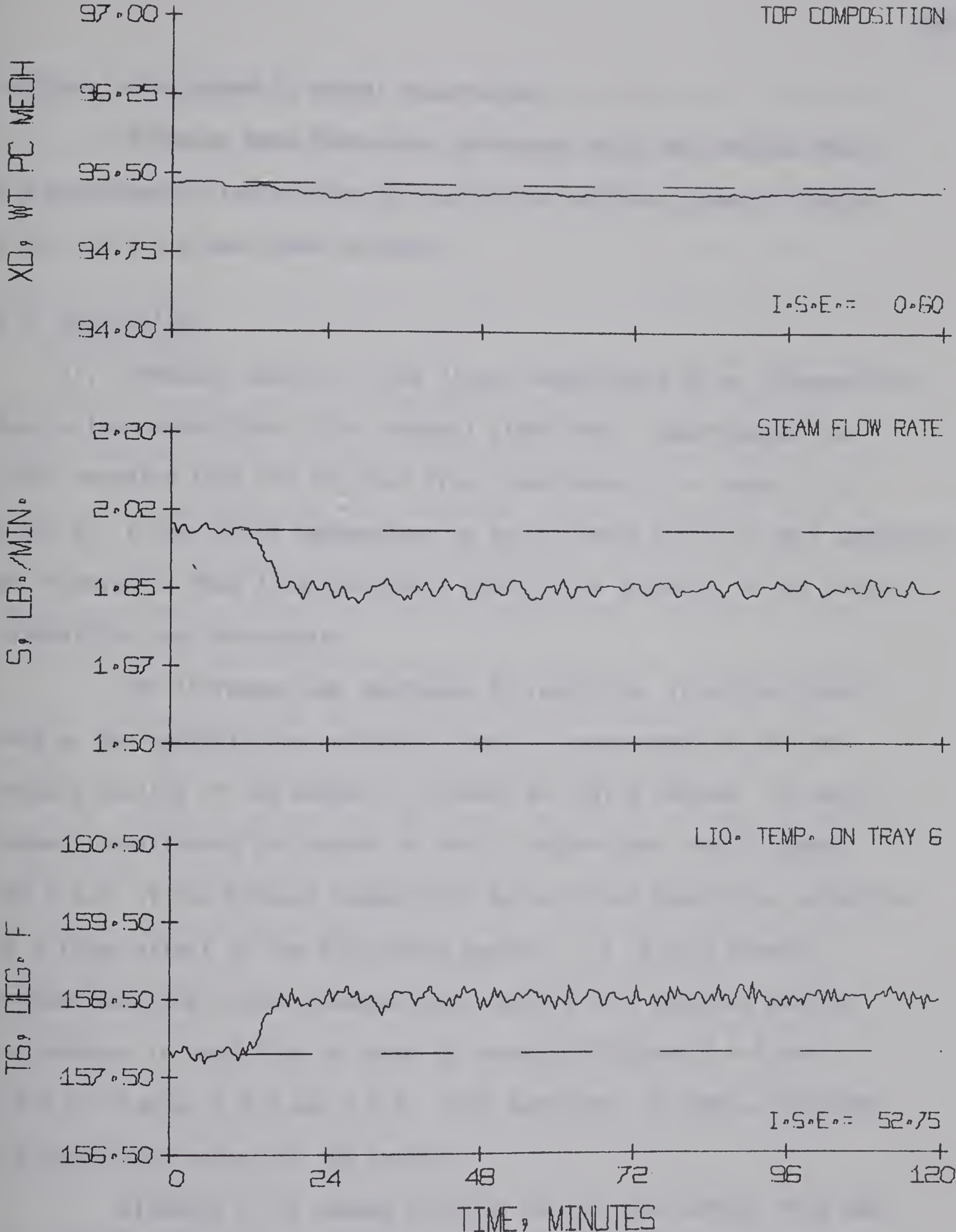


Figure 7.4-16 Feedback Control of the Liquid Temperature on Tray 6 by Manipulation of Steam Flow - Proportional Feedback Controller (50% - 30% step change in feed flow)

settings were judged by visual observation.

Although many tests were performed, only the results from the experimental tests using the controller settings given in Tables 7.4-1 and 7.4-2 have been included.

7.5 Discussion

(i) Feedback control of the liquid temperature on an intermediate tray using proportional plus integral algorithm ÷ Experimental results revealed that for all four trays considered, i.e. trays 1, 6, 7 and 8, if the liquid temperature on any of these trays is kept constant, an increase in feed flow rate would result in a decrease in top product composition and vice-versa.

For increases and decreases in feed flow, if reflux flow is used as the manipulative variable, there is improvement in the top product quality if the sensor is located at tray 8 instead of tray 7. Indeed, positioning the sensor on tray 7 rather than tray 8 causes the I.S.E. of top product composition to more than double due primarily to a large offset in the distillate quality. It is also clearly evident that the column responds more rapidly to a decrease than to an increase in feed flow as shown by comparing Figures 7.4-1 and 7.4-2 or Figures 7.4-3 and 7.4-4. This behavior, no doubt, indicates the non-linear nature of the system.

Although it is common practice to have the control tray near the corrective medium, if overhead composition is the desired product and steam flow is used as the corrective medium, sometimes, it is

necessary to locate the sensor some distance from the steam flow. For this distillation column, locating the sensor at tray 1 would result in a large offset in the top product composition, as indicated by Figures 7.4-5 and 7.4-6, while selecting tray 6 as the control tray has the obvious advantage of reducing the offset in the overhead composition, as shown by Figures 7.4-7 and 7.4-8. In spite of the fact that tray 6 is located far from the steam control valve, the control of liquid temperature on tray 6 presented little difficulty since there is only small initial departure of the temperature from the desired value and no oscillatory action is present. This can be explained by the fact that the change in vapor flow rate is transmitted through the column so rapidly that the elapsed time between a change in steam flow leading to increased boil-up and the time at which the new vapor rate effects the liquid temperature on tray 6 is almost negligible.

(ii) Feedback control of the liquid temperature on an intermediate tray using a proportional control algorithm ÷ In most cases studied, by using a proportional controller, with proper controller settings, top product composition can be maintained almost constant as shown in Figures 7.4-9, 7.4-10 and 7.4-13 to 7.4-16. The lone exception is using tray 8 as the control tray. As can be seen from Figures 7.4-11 and 7.4-12, although the maximum proportional controller constant available using a single DDC loop was used (K_{pmax} = 256.0), it was impossible to reduce the top product composition offset to zero. It appears that this is due simply to the fact that a larger proportional

controller constant than available using a single DDC loop is necessary.

However, the control schemes using only a proportional controller are not practical since it is not always possible to determine the correct optimum controller settings so that no offset would result in the overhead composition. These settings depend upon the magnitude and direction of the upset, as can be readily appreciated by examining the proportional gain values in Table 7.4-2. These values varied depending upon increases and decreases in feed flow.

CHAPTER VIII

DISCUSSION AND CONCLUSIONS

The success of the prediction of the control performance of the distillation column depends upon the validity of the models used to describe the dynamics of the distillation process and other elements in the control loop such as the sensing device and the control valve.

It should be kept in mind that the use of linear models to represent the dynamics of a distillation column certainly has its limitations due to the non-linear behavior of the column. For instance, experimental data from the University of Delaware column revealed that a set of linear, perturbation-type differential equations can predict the unsteady-state performance of this column with reasonably good accuracy only if the magnitude of any perturbation is not larger than $\pm$ 10 per cent of its steady-state value. In the case of the University of Alberta distillation column a series of experimental tests would need to be performed to determine how large the magnitude of the disturbance can be for the column to still be considered as a linear system. The use of simple transfer functions such as those in Chapter 5 to represent the dynamics of the column for both increases and decreases in feed, reflux and steam flows is only justified when the departure from steady-state conditions is small enough that the column behaves as a linear system. In view of the large magnitudes of the disturbances in

the feed rate and the reflux or steam flow rate which occurs due to the necessary corrective action, the agreement between the simulation results and the experimental results may not be as satisfactory as would be expected. This results because with deviations of such large magnitudes, the distillation column can no longer be considered as a linear process.

Nevertheless, by comparing the simulation results with the experimental results, it appears that the predicted results would be good enough for most purposes, particularly for just comparing the performance of the column at different proposed locations. Indeed, results from Chapters 6 and 7 showed that the "optimum" tray location predicted by the simulation results is the same tray as indicated by the experimental work. The use of simple linear models would not predict the steady-state behavior correctly because of the non-linearities in the system, but this may not be important, since steady-state data can be predicted by routine methods such as tray-to-tray calculations.

To determine the best sensor location for any distillation column, it is necessary to have a careful specification of a goal for the separation involving product purities, the tolerances allowed in the product compositions, the type of sensing element, etc. It is almost impossible to give any firm general recommendations. However, simulation results from both columns investigated suggested the following conclusions; these should be capable of extrapolation to large columns:

(i) Every effort should be made to obtain a sensing element of high sensitivity, i.e. one which can measure the temperature (or composition) of nearly pure streams, and it should have a fast response to any sudden change in temperature (or composition) and is able to provide continuous measurements.

(ii) If such a sensing device is available, direct control of top product composition by manipulation of reflux flow or direct control of bottom product composition by manipulation of steam flow should be used since these control arrangements generally are very satisfactory from both dynamic and steady-state standpoints. In some columns, however, the large hold-up of the liquid in the reboiler and the reflux accumulator might have a de-stabilizing effect on the column as it tends to generate additional time delay in the control loop. In these cases, the dynamic advantages of these control schemes might not be so great, but unless the time delay is excessively large, direct measurement of the overhead and the bottom product composition is preferable in most cases, based on steady-state characteristics.

(iii) If top product composition is to be maintained constant using a sensing device of low sensitivity, measurement on an intermediate tray should be used. Use of the top tray, as the control tray, in conjunction with the manipulation of reflux flow is recommended in most cases as the process time delay and the steady-state error in the overhead composition would be minimum. In addition, the fluid flow lag can be minimized by locating the reflux flow control valve very

close to the top tray.

Should the sensing element be incapable of detecting small variations of the controlled variable in the top tray, it might be necessary to move the sensing point a few trays down the column. However, it should be kept in mind that if reflux flow is used as the manipulative variable, the advantage of a larger error signal will be counterbalanced by an instability induced through the fluid flow lags between the trays and by a large steady-state offset in the overhead composition.

It is often stated that a possible advantage of sampling near the feed tray is that changes in feed composition or feed flow rate are detected sooner and corrective action can start before off-specification products result. However, simulation results showed this advantage does not offset other disadvantages caused by locating the sensing element away from the ends.

(iv) If bottom product composition is to be controlled, then control by manipulation of reflux flow is not advisable. Indeed, the direct measurement of bottom product composition or the measurement of the liquid composition on an intermediate tray is unsatisfactory from a dynamic standpoing due to the wide separation between the sensing device and the controlled flow. Use of a tray near the reflux control valve, in general results in a large steady-state offset in the bottom product composition. Therefore, steam flow should be employed as the manipulative variable if bottom product composition is to be kept constant.

(v) Whenever a very large error signal for the temperature (or composition) controller is needed, then measurement on an intermediate tray far away from the ends of the column is required, steam flow should be used as the manipulative variable, since the disadvantage of locating the sensing point far away from the controlled flow would be less pronounced for boil-up control as the vapor flow lag is small and may be negligible compared with other lags in the control loop. Except with very large distillation columns, this flow lag is generally unnoticeable. The success of the control scheme using steam flow as the manipulative variable depends mainly on the dynamics of the reboiler since in general, the major lag comes from the reboiler itself.

(vi) To compare the performance of the column for different sensor locations, the determination of the effective time delay due to the fluid flow lag is of prime importance. Since the time constants in the transfer functions representing the dynamics of the column are about the same for any control point, the control behavior depends mainly on the time delay in the control loop. Careful studies should be conducted to evaluate the effective time delay due to the fluid flow lag to permit better prediction of the controllability of the column at different control points. It should be mentioned here that the time delay determined by the Oldenburg and Sartorius method or simply by visual observation might not be satisfactory since it is possible that this time delay might not accurately describe the true fluid flow lag in the column, and therefore, erroneous conclusions

about the column performance might result.

In addition, in many actual systems, the use of the sensing device and the control valve would introduce some dynamic lag in the system. These lags would need to be determined as accurately as possible.

(vii) If direct measurement of top and bottom product composition is employed, and time delay and other lags are present in the control loop, combined feedforward-feedback control is very helpful in damping out oscillatory behavior and reducing the maximum overshoot.

However, feedforward plus feedback control of the liquid temperature (or composition) on an intermediate tray is seldom necessary since there is little improvement in product quality.

(viii) Feedback control of the liquid temperature on an intermediate tray using a proportional control only so that there is no composition offset in one of the product streams is desirable but not very practical since this control arrangement suffers from the drift in the product quality caused by imperfect modelling and secondary disturbances in the process.

Finally, the following summary gives some guidelines which might be useful in selecting the control tray:

- The control tray should be one where easy measurements of changes in temperature (or composition) is possible in the absence of control.

- The tray should be where a constant liquid temperature (or

composition) on this tray ensures a satisfactory product quality. Wood's method of tray-to-tray calculations proved very valuable to determine the location of this tray.

- The tray should be chosen so that the hydrodynamic delay should be as small as possible.

- The tray should be chosen so that if the liquid temperature (or composition) on this tray is maintained constant, the column tends as fast as possible to the desired steady-state in the absence of further disturbances. In the presence of continued disturbances, the column departs as little as possible from the desired steady-state. Rosenbrock's method (64) can be used to determine the location of the tray with these characteristics.

None of these guidelines can be applied without due regard for the others and the final choice of the sensing location depend on the information available and engineering judgement.

BIBLIOGRAPHY

1. Anisimov, I.V., "A Study of the Dynamic and Static Characteristics of the Process of Fractionation Distillation", Automatic and Remote Control, Proc. IFAC Basle, 2, 300-308, (1963).

2. Archer, D.H., "An Optimising Control for the Chemical Process Industries", Brit. Chem. Eng., 5, 88-94, (1960).

3. Armstrong, W.D., and Wood, R.M., "An Introduction to the Theoretical Evaluation of the Frequency Response of a Distillation Column to a Change in Reflux Flow Rate", Trans. Instn. Chem. Engrs., 39, 80-90, (1961).

4. Auns, J., "Effect of Sensor Location on Binary Distillation Control", M.Sc. Thesis, Department of Chemical Engineering, University of Ottawa, (1966).

5. Ausman, J.S., "Amplitude Frequency Response Analysis and Synthesis of Unfactored Transfer Function", Trans. of ASME, Journal of Basic Engineering, 86, 32-34, March, 1964.

6. Baber, M.F., Edwards, L.L. Jr., Harper, W.T., Jr. Witter, M.D., and Gerster, J.A., "Experimental Transient Response of a Pilot Plant Distillation Column", Chem. Eng. Prog. Symp. Ser., 57, No. 36, 148-159, (1961).

7. Baber, M.F., and Gerster, J.A., "Experimental Transient Response of a Pilot Plant Distillation Column. Part II - Response to Liquid and Vapor Rate Perturbations", AIChE Journal, 8, No. 3, 407-415, (1962).

8. Bailey, R.V., and Law, V.J., "A Method for the Determination of Approximate System Transfer Functions", Chem. Eng. Sci., 18, 189-202, (1963).

9. Bauer, R.L., and Orr, C.P., "Distillation Control Problem, Application of the McCabe-Thiele Diagram", Chem. Eng. Prog., 50, No. 6, 312-319, (1954).

10. Berger, D.E., and Campbell, G.G., "Experience in Controlling a Large Separation Column with a Continuous Infrared Analyzer", Chem. Eng. Prog. 51, 348-352, (1955).

11. Berry, M.W., "Gas Chromatograph Operating Manual", Department of Chemical and Petroleum Engineering, University of Alberta, (1970).

12. Berry, M.W., "Implementation and Evaluation of Two-Point Distillation Control Scheme", M.Sc. Thesis, Department of Chemical and Petroleum Engineering, University of Alberta, (1971).

13. Berry, M.W., and Pacey, W.C., "Distillation Column Data - Transient Response via Pulse Testing", Department of Chemical and Petroleum Engineering, University of Alberta, (1969).

14. Bertrand, L., and Jones, J.B., "Controlling Distillation Columns", Chem. Eng., 68, 139-144, Feb. 20, 1961.

15. Bornard, G., Duthatel, G., Melennec, J.L., and Sempe, B., "Closed Loop Predictive Digital Control of the Industrial Distillation Column", Paper presented at the 4th IFAC Congress, Warszawa, June, 1969.

16. Boyd, D.M., Jr., "Fractionation Instrumentation and Control - Part I", Petrol. Ref., 27, No. 10, 533-536, (1948).

17. Boyd, D.M. Jr., "Fractionation Instrumentation and Control - Part II", Petrol. Ref., 27, No. 11, 594-597, (1948).

18. Brownlee, K.A., "Statistical Theory and Methodology in Science and Engineering", John Wiley and Sons Inc., New York, (1960).

19. Buckley, P.S., "Techniques of Process Control", John Wiley and Sons Inc., New York, (1964).

20. Bui-Minh, C., "Distillation Column Data-Transient Response via Control of the Liquid Temperature on an Intermediate Tray", Department of Chemical and Petroleum Engineering, University of Alberta, (1971).

21. Cardenas, E.I., "The Effects of Feed Composition on the Location of the Temperature Control Points in a Continuous Distillation Column", M.Sc. Thesis, Department of Chemical Engineering, University of Colorado, (1964).

22. Chen, C.F., and Philip, P.L., "Graphical Determination of Transfer Function Coefficients of a System from its Frequency Response", AIEE Trans., Part II (Applications and Industry), 82, 42-45, March, 1963.

23. Chen, C.F., and Haas, I.J., "Elements of Control System Analysis", Prentice-Hall Inc., New Jersey, (1968).

24. Dudnikov, E.E., "Determination of Transfer Function Coefficients of a Linear System from the Initial Portion of an Experimentally Obtained Amplitude Phase Characteristic", Automat. Remote Contr., 20, 552-558, May, 1959.

25. Fenske, E.R., and Broughton, D.B., "Fractionation of Mixed Aromatics from Udex Extractions", Ind. Eng. Chem., 47, No. 4, 714-717, (1955).

26. Fletcher, R., and Powell, M.J.D., "A Rapidly Convergent Descent Method for Minimization", Computer Journal, 6, 163-168, (1963).

27. Fletcher, R., "Function Minimization Without Evaluating Derivatives", Computer Journal, 8, 33-41, (1965).

28. Ganapathy, S., and Krishna, G., "A Method of Determining the Transfer Function of a Linear System in Terms of its Poles and Zeros from the Frequency Response", AIEE Trans., Part II (Applications and Industry), 81, 282-290, Nov. 1962.

29. Harriot, P., "Process Control", McGraw-Hill Book Co., New York, (1964).

30. Heidemann, R.A., "An Optimal Discrete Controller for a System with Load Changes", Joint Automatic Control Conference, 8th., 452-464, (1967).

31. Holland, C.D., "Unsteady State Processes with Applications in Multicomponent Distillation", Prentice-Hall Inc., New Jersey, (1966).

32. Hoyt, P.R., and Stanton, B.D., "Analyzing Process Control Systems", Petrol. Ref., 32, No. 10, 115-119, (1953).

33. International Business Machines Corp., "System/360 Continuous System Modeling Program", File No. 360A-CX-16X, User's Manual, Form. H20-0367-2.

34. International Business Machines Corp., "System / 360 Continuous System Modeling Program", File No. 360A-CX-16X, Application Description, Form. H20-0240-2.

35. Izawa, K., and Morinaga, T., "Dynamic Characteristics of Binary Distillation Column", Automatic and Remote Control, Proc. IFAC Basle, 2, 229-237, (1963).

36. Klein, V., "The Identification of Linear System with a Given Structure by Means of Frequency Responses", Automatic and Remote Control, Proc. IFAC London, Paper 46.A, June 1966.

37. Levy, E.C., "Complex Curve Fitting", Institute of Radio Engineers, Transactions on Automatic Control, AC-4, 37-43, May, 1959.

38. Lupfer, D.E. and Oglesby, M.W., "Automatic Control of Distillation Columns", Ind. Eng. Chem., 53, No. 12, 963-969, (1961).

39. Lupfer, D.E., and Johnson, M.L., "Automatic Control of Distillation Columns to Achieve Optimum Operation", ISA Trans., 3, No. 2, 1965-174, (1964).

40. Luyben, W.L., Verneuil, V.S., Jr., and Gerster, J.A., "Transient Response of Ten-Tray Distillation Column-Complete Data and Results", Department of Chemical Engineering, University of Delaware, August, 1963.

41. Luyben, W.L., and Gerster, J.A., "Feedforward Control of Distillation Columns", Ind. Eng. Chem., Process Design and Development, 3, No. 4, 374-381, (1964).

42. Luyben, W.L., Verneuil, V.S., Jr., and Gerster, J.A., "Experimental Transient Response of a Pilot Plant Distillation Column. Part IV - Response of a Ten-Tray Column", AIChE Journal, 10, No. 3, 357-364, (1964).

43. Luyben, W.L., "10 Schemes to Control Distillation Columns with Sidestream Drawoff", ISA Journal, 13, No. 7, 37-43, (1966).

44. Luyben, W.L., "Distillation, Feedforward Control with Intermediate Feedback Control Trays", Chem. Eng. Sci., 24, No. 6, 997-1007, (1969).

45. Luyben, W.L., "Feedback Control of Distillation Column by Double Differential Temperature Control", Ind. Eng. Chem. Fund., 8, No. 4, 739-744, (1969).

46. Marino, P.A., and Stutzman, L.F., "Distillation Column Dynamics with the Use of Pulse Technique", AIChE Journal, 12, No. 3, 603-604, May 1966.

47. Mickley, H.S., Sherwood, T.S., and Reed, C.E., "Applied Mathematics in Chemical Engineering", McGraw-Hill Book Co., New York, (1957).

48. Mitchell, D.S., and Webb, C.R., "A Study of Interaction in a Multiloop Control System", Automatic and Remote Control, Proc. IFAC London, 1, 142-152, (1960).

49. Moczek, J.S., Otto, R.E., and Williams, T.J., "Approximation Models for the Dynamic Response of Large Distillation Columns", Automatic and Remote Control, Proc. IFAC Basle, 2, 238-248, (1963).

50. Oldenbourg, R.C., and Sartorius, H., "The Dynamics of Automatic Control", American Society of Mechanical Engineers, New York, (1948).

51. Pacey, W.C., "Distillation Column Operating Manual", Department of Chemical and Petroleum Engineering, University of Alberta, (1970).

52. Pacey, W.C., "Distillation Column Feedforward and Feedback Control Scheme", M.Sc. Thesis, Department of Chemical and Petroleum Engineering, University of Alberta, (1971).

53. Parkins, R., "Continuous Distillation Plant Controls", Chem. Eng. Prog., 55, No. 7, 60-68, (1959).

54. Phister, M. Jr., "Application of Digital Systems to Process Control", Chem. Eng. Prog., 54, No. 9, 53-58, (1958).

55. Powell, M.J.D., "An Efficient Method for Finding the Minimum of a Function of Several Variables without Calculating Derivatives", Computer Journal, 6, 155-162, (1964).

56. Powell, M.J.D., "A Method for Minimizing a Sum of Squares of Non-Linear Functions without Calculating Derivatives", Computer Journal, 7, 303-307, (1965).

57. Pyle, C., "Control Systems for Distillation Towers", The Oil and Gas Journal, 47, 97-103, Oct. 13, 1949.

58. Rees, N.W., "Dynamic Identification and Optimum Control Studies on a Pilot Distillation Column", Automatic and Remote Control, Proc. IFAC Moscow, Paper 32-C, (1960).

59. Robinson, C.S., and Gilliland, E.R., "Elements of Fractional Distillation", McGraw-Hill Book Co., New York, (1950).

60. Rose, A., and Williams, T.J., "Automatic Control in Continuous Distillation", Ind. Eng. Chem., 47, No. 11, 2284-2289, (1955).

61. Rosenbrock, H.H., "Calculation of the Transient Behaviour of Distillation Columns", Brit. Chem. Eng., 3, 364-467, 432-435, 491-494, (1958).

62. Rosenbrock, H.H., Tavendale, A.B., Storey, C. and Challis, J.A., "Transient Behaviour of Multicomponent Distillation Columns", Automatic and Remote Control, Proc. IFAC Moscow, 1277-1282, (1960).

63. Rosenbrock, H.H., "An Automatic Method for Finding the Greatest or Least Value of a Function", Computer Journal, 3, 175-184, (1960).

64. Rosenbrock, H.H., "The Control of Distillation Columns", Trans. Instn. Chem. Engrs., 40, 35-53, (1962).

65. Rosenbrock, H.H., and Storey, C., "Computation Techniques for Chemical Engineers", Pergamon Press, New York, (1966).

66. Russel, D.W., and Weaver, C.H., "Synthesis of Closed Loop Systems using Curvilinear Squares to Predict Root Location", AIEE Trans., Part II (Applications and Industry), 71, 95-104, Jan. 1952.

67. Sanathanan, C.K., and Koerner, I., "Transfer Function Synthesis as a Ratio of Two Complex Polynomials", IEEE Trans. on Automatic Control, AC-8, 56-58, Jan. 1963.

68. Shinskey, F.G., "Feedforward Control of Distillation Columns", The Oil and Gas Journal, 63, 97-102, April 12, 1965.

69. Sproul, J.S., and Gerster, J.A., "Experimental Transient Response of a Pilot Plant Distillation Column, Part III - Condensing and Reboiling Systems", Chem. Eng. Prog. Symp. Ser., 59, No. 46, 21-31, (1965).

70. Staffin, H.K., and Staffin, R., "Approximating Transfer Functions from Frequency Response Data", Instrum. Contr. Syst., 38, 137-144, Feb. 1965.

71. Strobel, H., "On a New Method of Determining the Transfer Function by Simultaneous Evaluation of the Real and Imaginary Parts of the Measured Frequency Response", Automatic and Remote Control Proc. IFAC London, Paper 1F, (1966).

72. Summer, A., "A Method of Fitting Rational Transfer Functions to Frequency Responses", Proc. Instn. Mech. Engrs., 179, 132-137, (1964).

73. Svrcek, W.Y., "Binary Distillation Column Dynamics", Ph.D. Thesis, Department of Chemical and Petroleum Engineering, University of Alberta, (1967).

74. Tivy, V.V. St. L., "Automatic Control of Fractionating Columns", Petrol. Ref. 27, No. 11, 603-608, (1948).

75. Uitti, K.D., "The Effects of Control Point Location Upon Column Control", Petrol. Ref., 29, No. 3, 130-134, (1950).

76. Wherry, T.C., and Berger, D.E., "What's New in Fractionator Control?", Petrol. Ref., 37. No. 5, 221-224, (1958).

77. Wilde, D.J., "Optimum Seeking Methods", Prentice-Hall, Inc., New Jersey, (1964).

78. Wilkinson, W.L., and Armstrong, W.D., "An Approximate Method of Predicting Composition Response of a Fractionating Column", Chem. Eng. Sci., 7, 1-7, (1957).

79. Williams, T.J., Harnett, R.T., and Rose, A., "Automatic Control in Continuous Distillation Column", Ind. Eng. Chem., 48, 1008-1019, (1956).

80. Williams, T.J., Harnett, R.T., "Automatic Control in Continuous Distillation Column", Chem. Eng. Progr., 53, No. 5, 220-225, May, 1957.

81. Williams, T.J., "Instrumentation and Control of Distillation Columns", Ind. Eng. Chem., 50, No. 9, 1214-1221, (1958).

82. Williams, T.J., "Process Control", Chem. Eng., 67, No. 7, 119-124, July 25, 1960.

83. Williams, T.J., "The Status of Studies of the Dynamics of Mass-Transfer Operations - A Review and Commentary", Chem. Eng. Prog. Symp. Ser., 59, No. 46, 1-8, (1963).

84. Wood, C.E., "Tray Selection for Column Temperature Control", Chem. Eng. Prog., 64, No. 1, 85-88, (1968).

85. Wood, R.K., and Pacey, W.C., "Experimental Evaluation of Feed-back, Feedforward and Combined Feedforward-Feedback Binary Distillation Column Control", Paper presented at the 20th Canadian Chemical Engineering Conference, Sarnia, Oct. 19-22, 1970.

NOMENCLATURE

The nomenclature which appears at only one location in the thesis is defined at that point and does not appear in this list.

(a) Mathematical Symbols

C_i	liquid composition (or temperature) on tray i
D	distillate flow rate
F	feed flow rate
G_C	feedback controller transfer function
G_{FF}	feedforward controller transfer function
G	transfer function of process
G_{DL}	$X_D(s)/L(s)$
G_{DR}	$X_D(s)/R(s)$
D_{DV}	$X_D(s)/V(s)$
G_{iL}	$C_i(s)/L(s)$
G_{iR}	$C_i(s)/R(s)$
G_{iV}	$C_i(s)/V(s)$
G_R	transfer function for the reboiler
G_V	transfer function for the control valve
G_{WL}	$X_W(s)/L(s)$
G_{WR}	$X_W(s)/R(s)$
G_{WV}	$X_W(s)/V(s)$
H_D	transfer function for the overhead composition sensing element

H_i	transfer function for the sensing element used to measure the liquid temperature (or composition) on intermediate tray i
H_W	transfer function for the bottom product composition sensing element
K	proportional gain of the transfer function G
K_c	feedback controller gain
K_{FF}	feedforward controller gain
K_p	DDC proportional controller gain
L	load
n	total number of trays in a distillation column
R	reflux flow
(s)	Laplace transform operator
S	steam flow
t	time
T_i	temperature of the liquid on tray i
V	boil-up rate
X_D	top product composition
X_F	feed composition
X_i	liquid composition on intermediate tray i
X_W	bottom product composition
τ_1, τ_2, τ_3	time constant
τ_D	time delay
τ_I	integral time of the feedback controller

ω	frequency
Δt	DDC sampling time

(b) Abbreviations

Comp.	Composition
Deg.	Degree
I.S.E.	Integral of the squared error
Liq.	Liquid
M.D.	Maximum deviation
MEOH	Methanol
Off.	Offset
pc	per cent
S.T.	Settling time
Temp.	Temperature
ppm	part per million

CONTROL SCHEME SYMBOLS

FR	Flow Recorder
FRC	Flow Recorder Controller
GC	Gas Chromatograph
LIC	Level Indicator Controller
PIC	Pressure Indicator Controller
TRC	Temperature Recorder Controller
——	Process
—⊗	Measurements
----	Analog Control Lines
—·—	Computer Control Lines
	Control Valve

APPENDIX A

COMPARISON OF EXPERIMENTAL DATA WITH THE PROPOSED MODELS

A.1 Comparison of Experimental Data with the Proposed Models for the University of Delaware Distillation Column

A typical list of steady-state operating conditions for the University of Delaware column is given in Table A.1-1.

Figures A.1-1 to A.1-18 are plots of the change of top product composition, bottom product composition and the liquid composition on intermediate trays 1, 3, 7, 9 of this column for a step change in feed composition, reflux flow and reboil vapor rate. The points are the experimental values and the solid lines represent the data as predicted by the models used in this work.

Figures A.1-1 to A.1-6 show the transient response of this column for Run No. 8 where feed composition was increased by 8.2 mole per cent acetone, Figures A.1-7 to A.1-12 give the transient response for Run No. 6-V where reflux flow was increased by 13.7 per cent and Figures A.1-13 to A.1-18 are the transient response of this column for Run No. 10-V where reboil vapor rate was increased by 6.7 per cent from its initial steady-state value.

Steady-state data for each of these runs (8,6-V and 10-V) are available in Reference (40). All run numbers in section A.1 were designated by Gerster et al (40).

Table A.1-1

Typical Steady-State Conditions of the

University of Delaware Distillation Column

(Run No. 8)

Feed flow rate	1.4932 lb.mole/min.
Reflux flow rate	0.9235 lb.mole/min.
Boil-up flow rate	2.2300 lb.mole/min.
Top product flow rate	0.8276 lb.mole/min.
Bottom product flow rate	0.6652 lb.mole/min.
Feed composition	48.0 mole % acetone
Top product composition	79.2 mole % acetone
Bottom product composition	8.1 mole %acetone
Composition of the liquid on tray 1	11.4 mole % acetone
Composition of the liquid on tray 2	20.0 mole % acetone
Composition of the liquid on tray 3	29.5 mole % acetone
Composition of the liquid on tray 4	36.8 mole % acetone
Composition of the liquid on tray 5	43.2 mole % acetone
Composition of the liquid on tray 6	44.6 mole % acetone
Composition of the liquid on tray 7	49.2 mole % acetone
Composition of the liquid on tray 8	54.9 mole % acetone
Composition of the liquid on tray 9	61.8 mole % acetone
Composition of the liquid on tray 10	70.2 mole % acetone
Pressure in the condenser	39.7 psia
Feed temperature	100.0°F
Reflux temperature	94.0°F

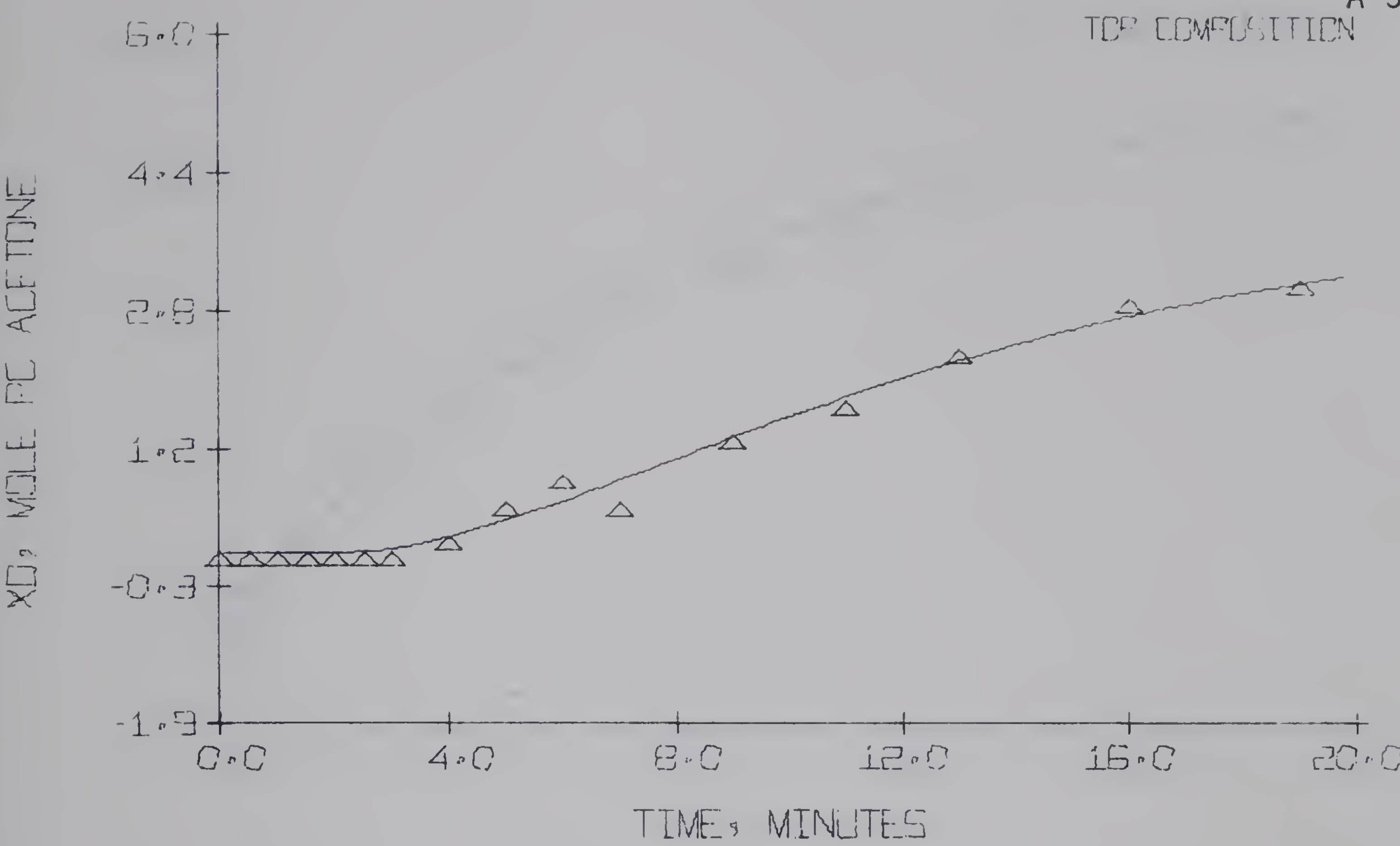


Figure A.1-1

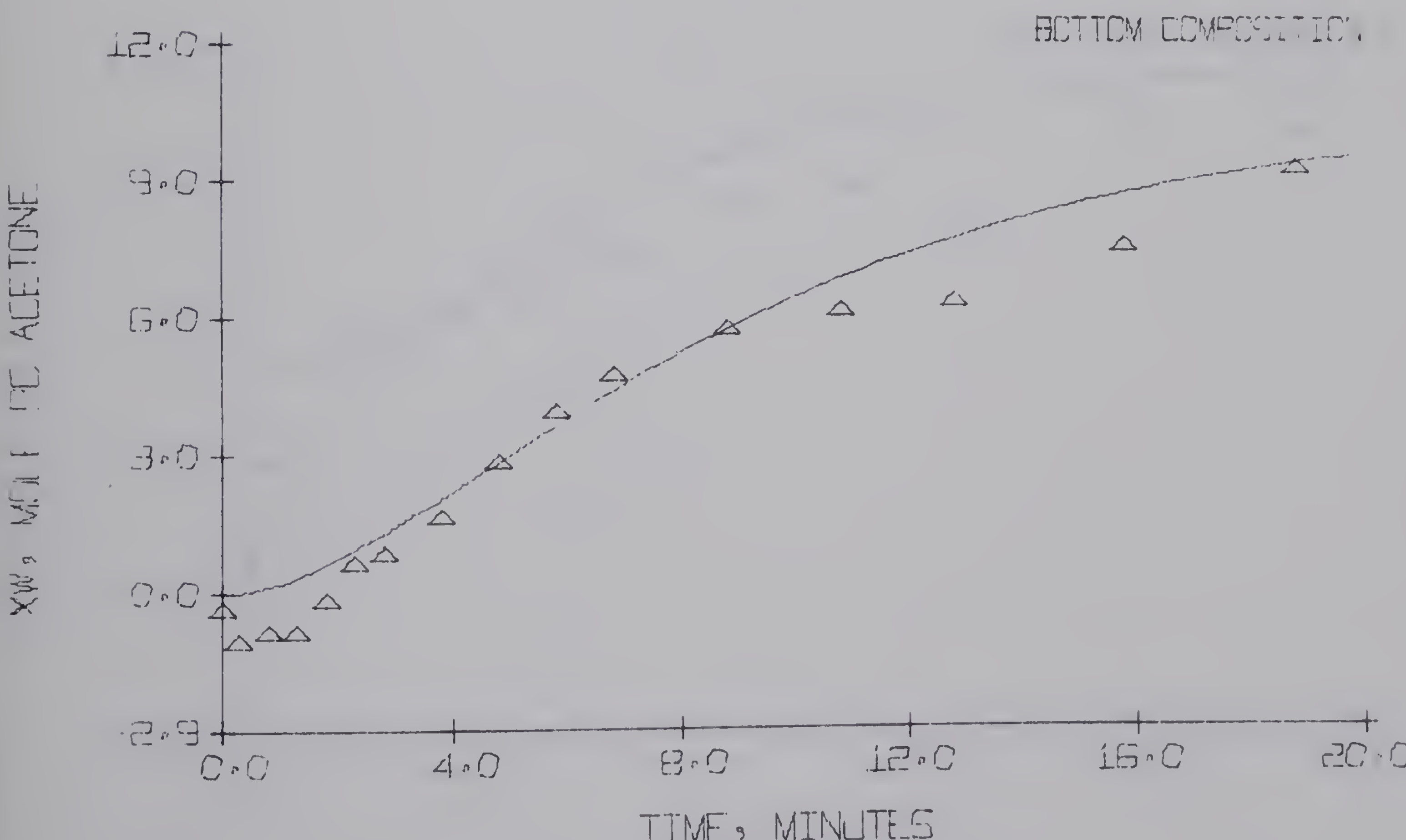
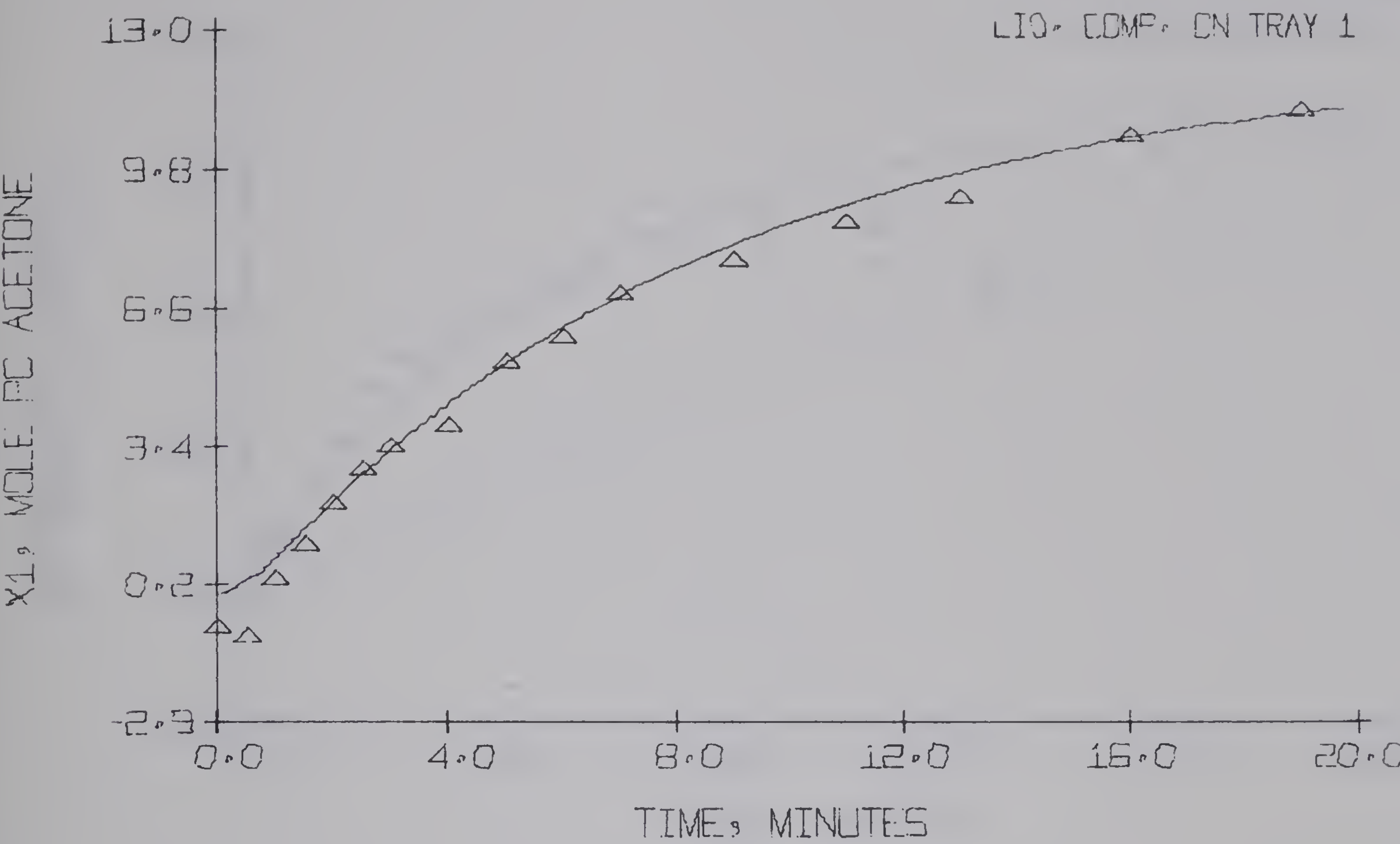


Figure A.1-2



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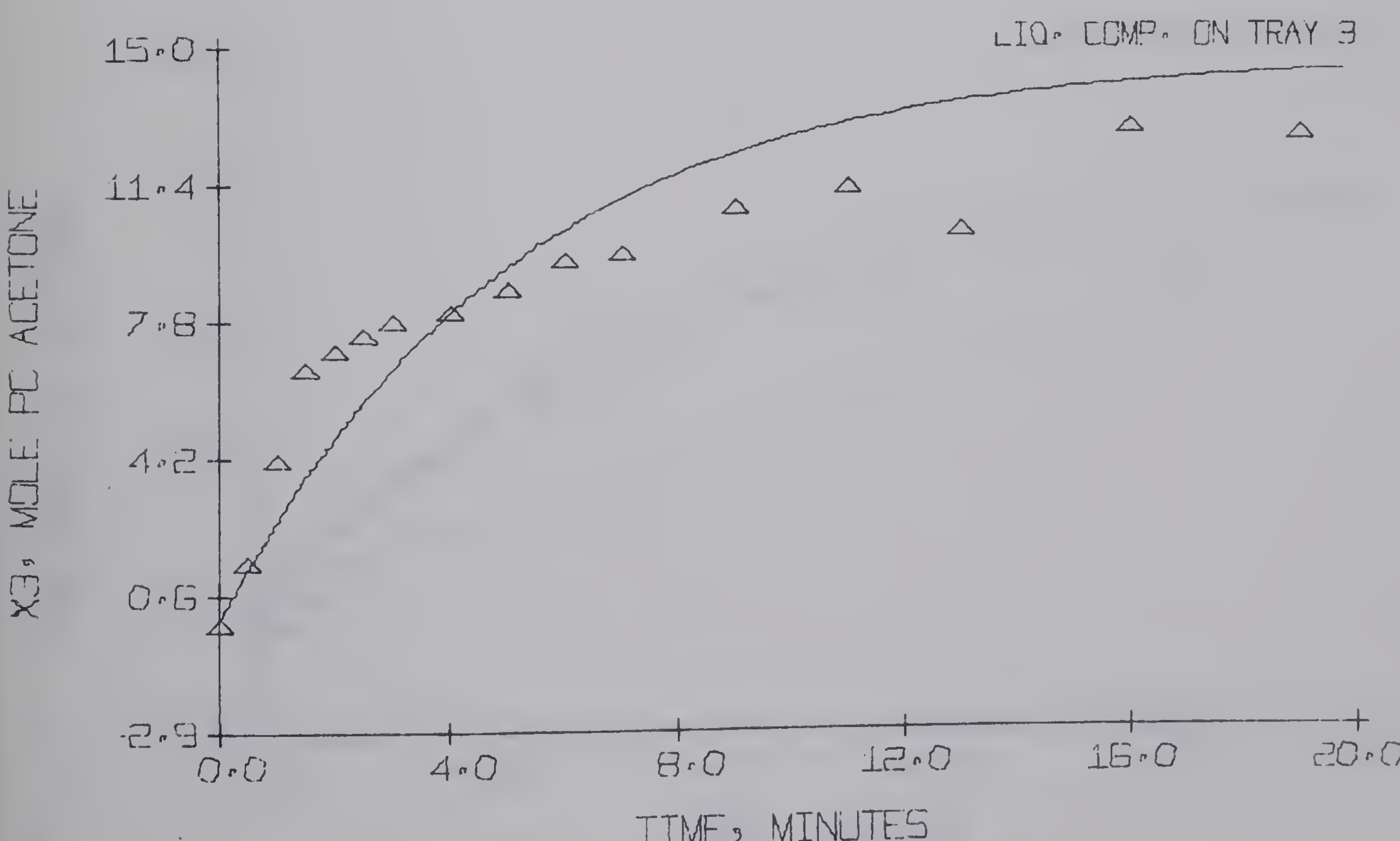

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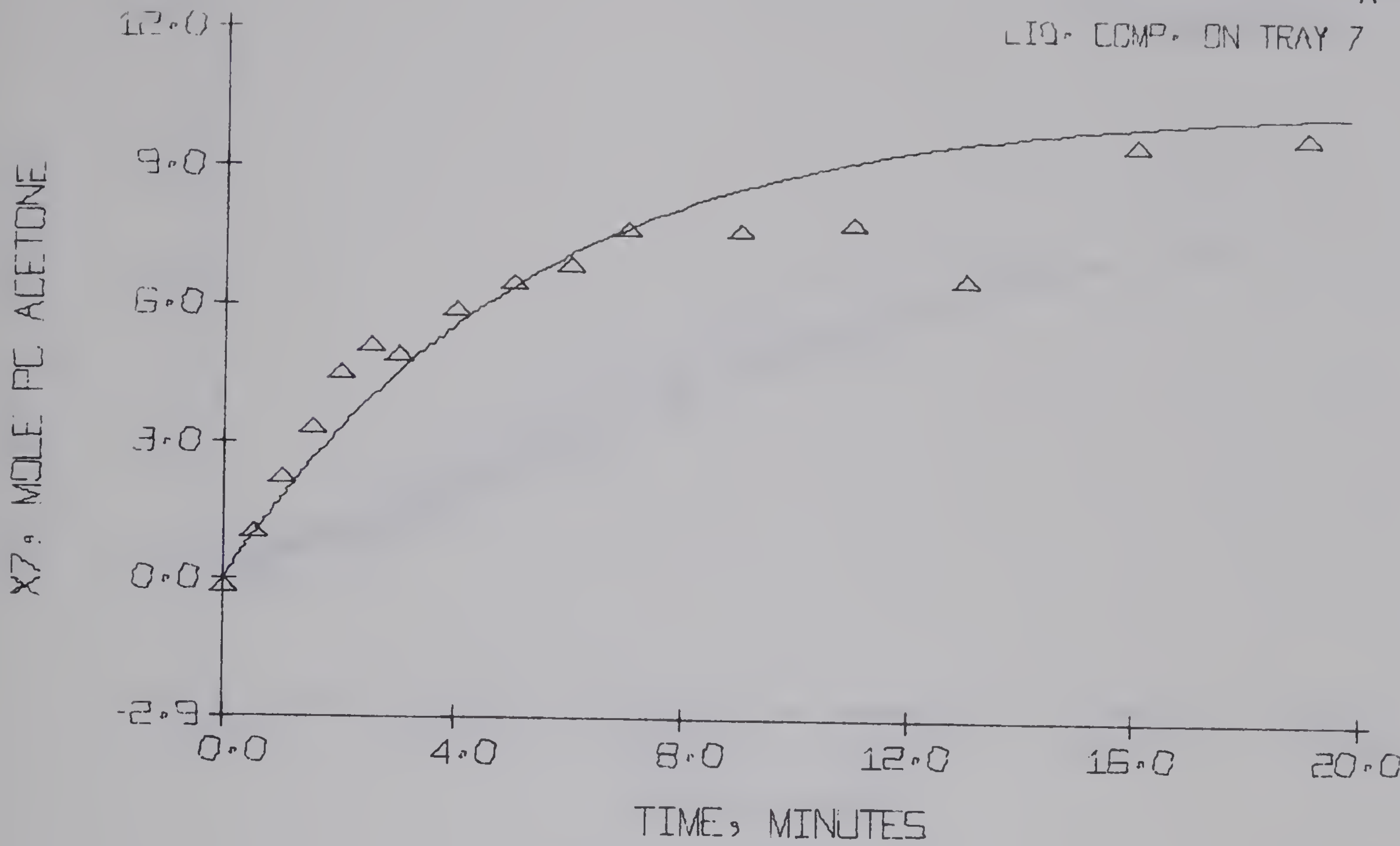

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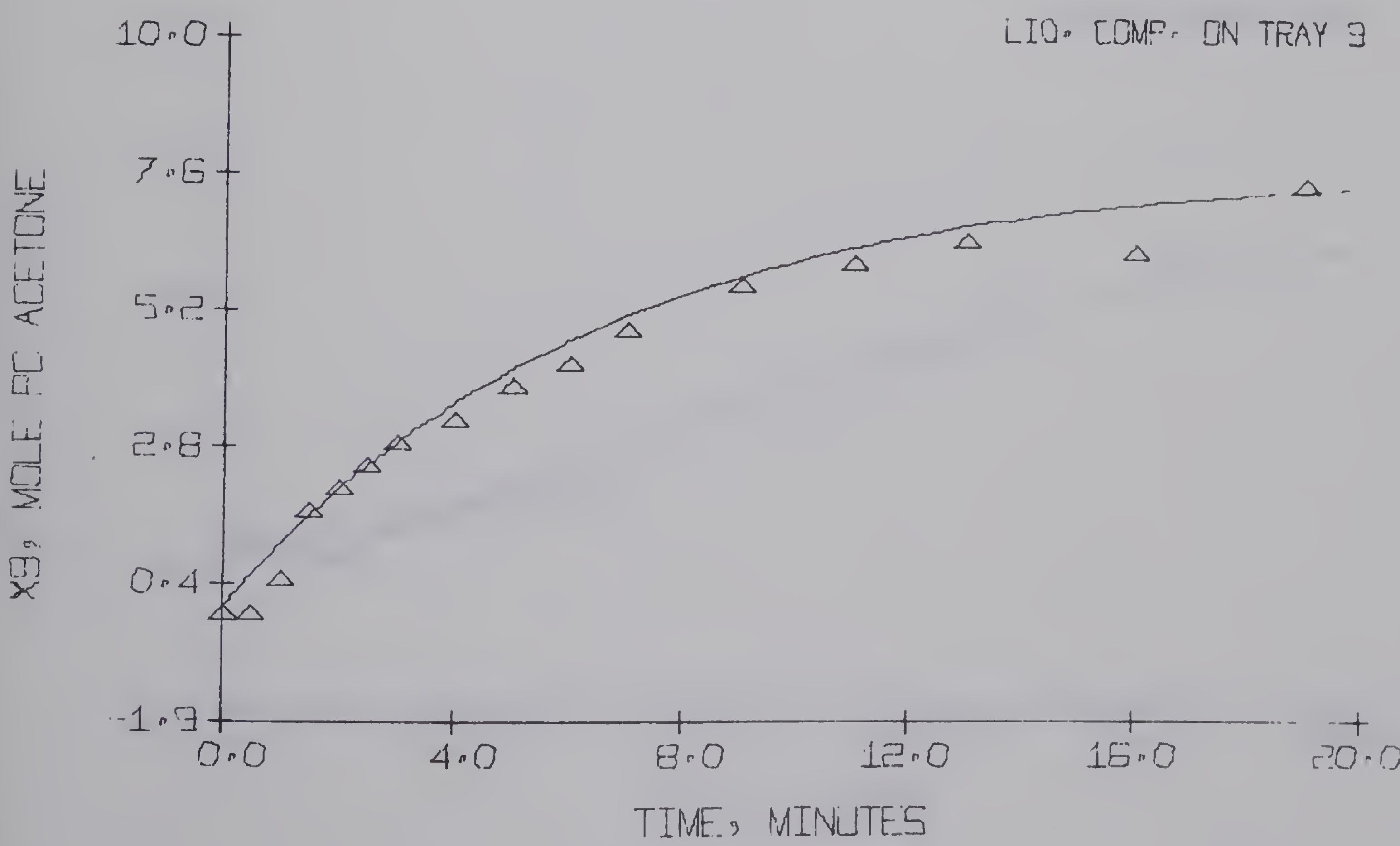

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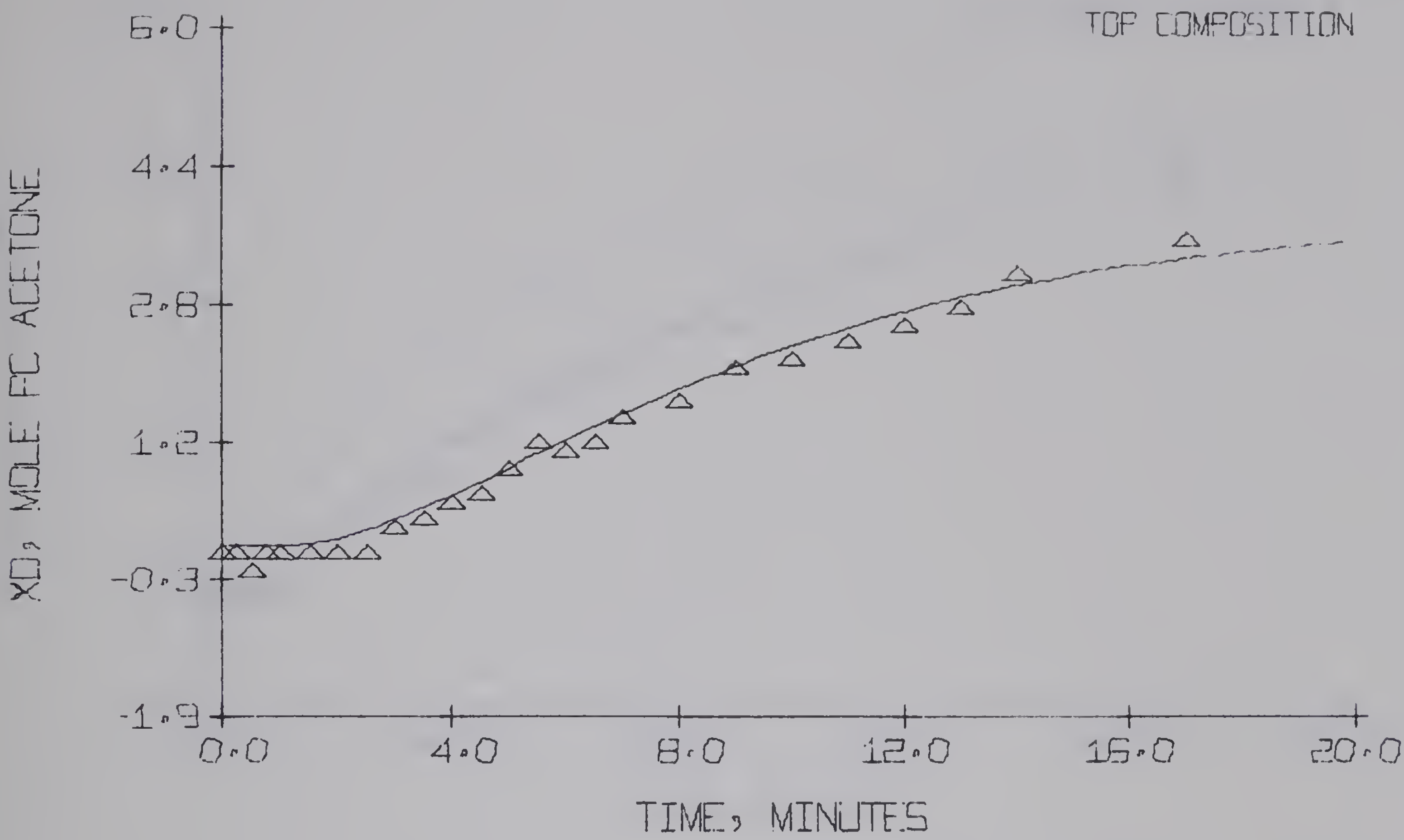

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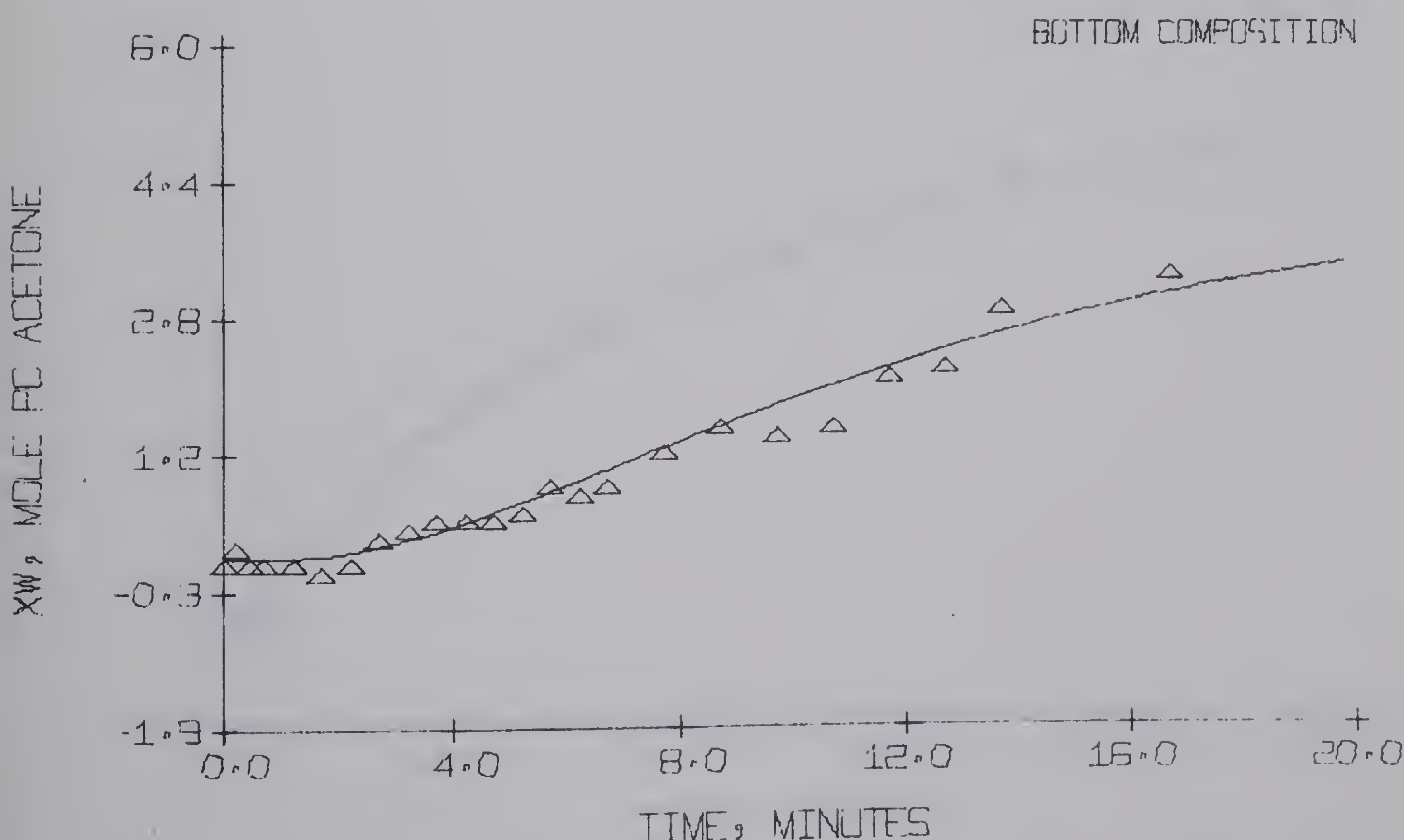

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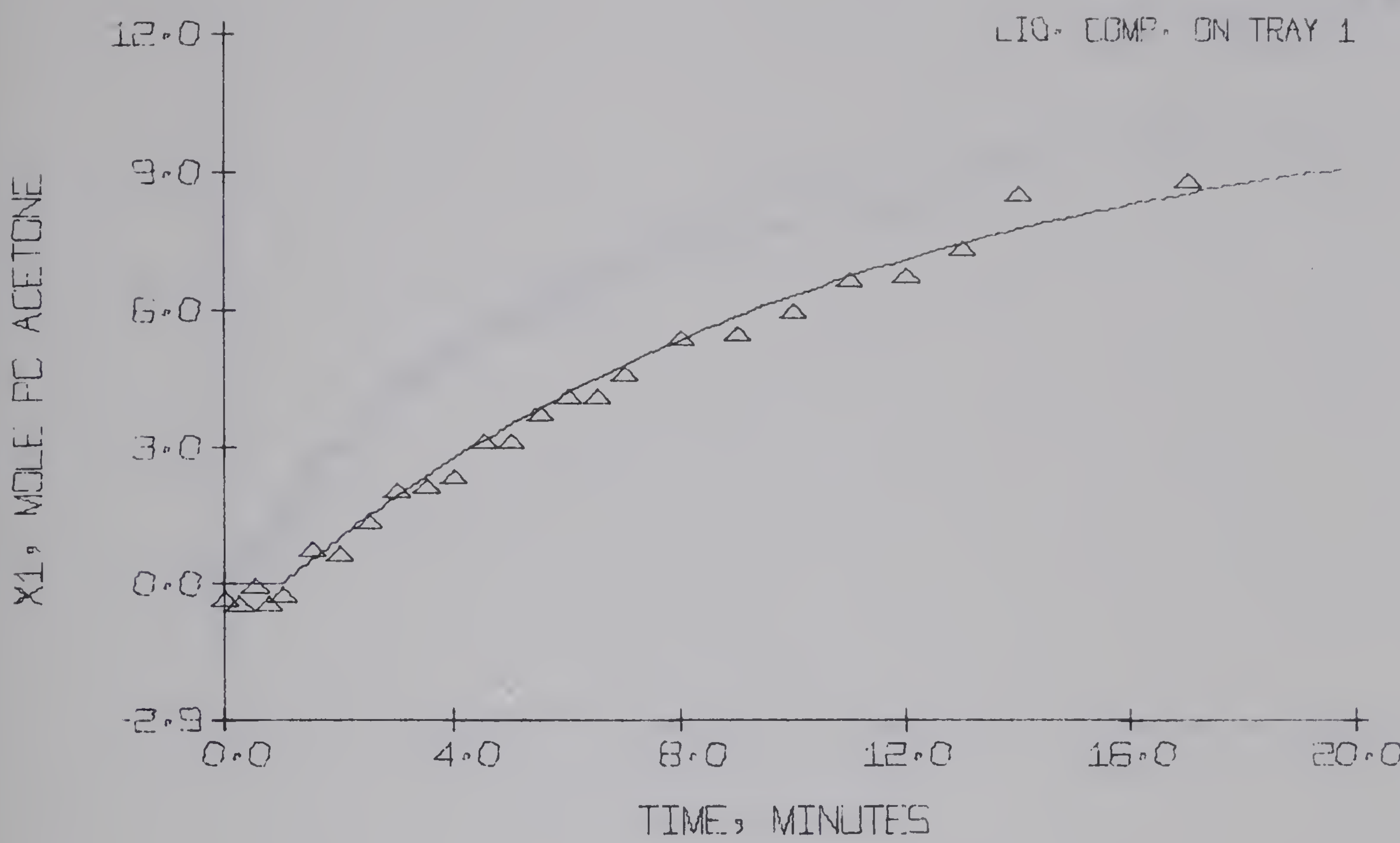

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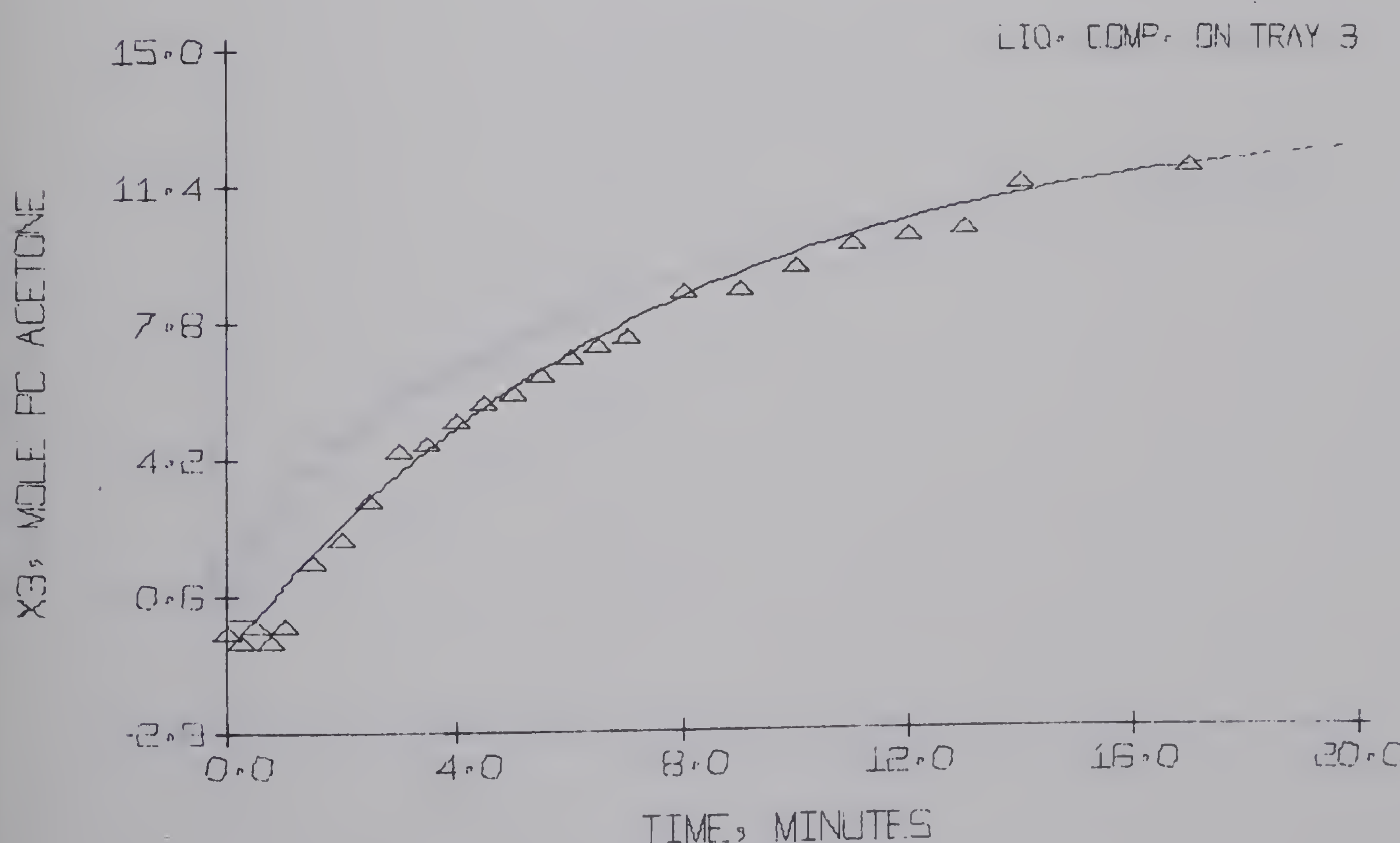

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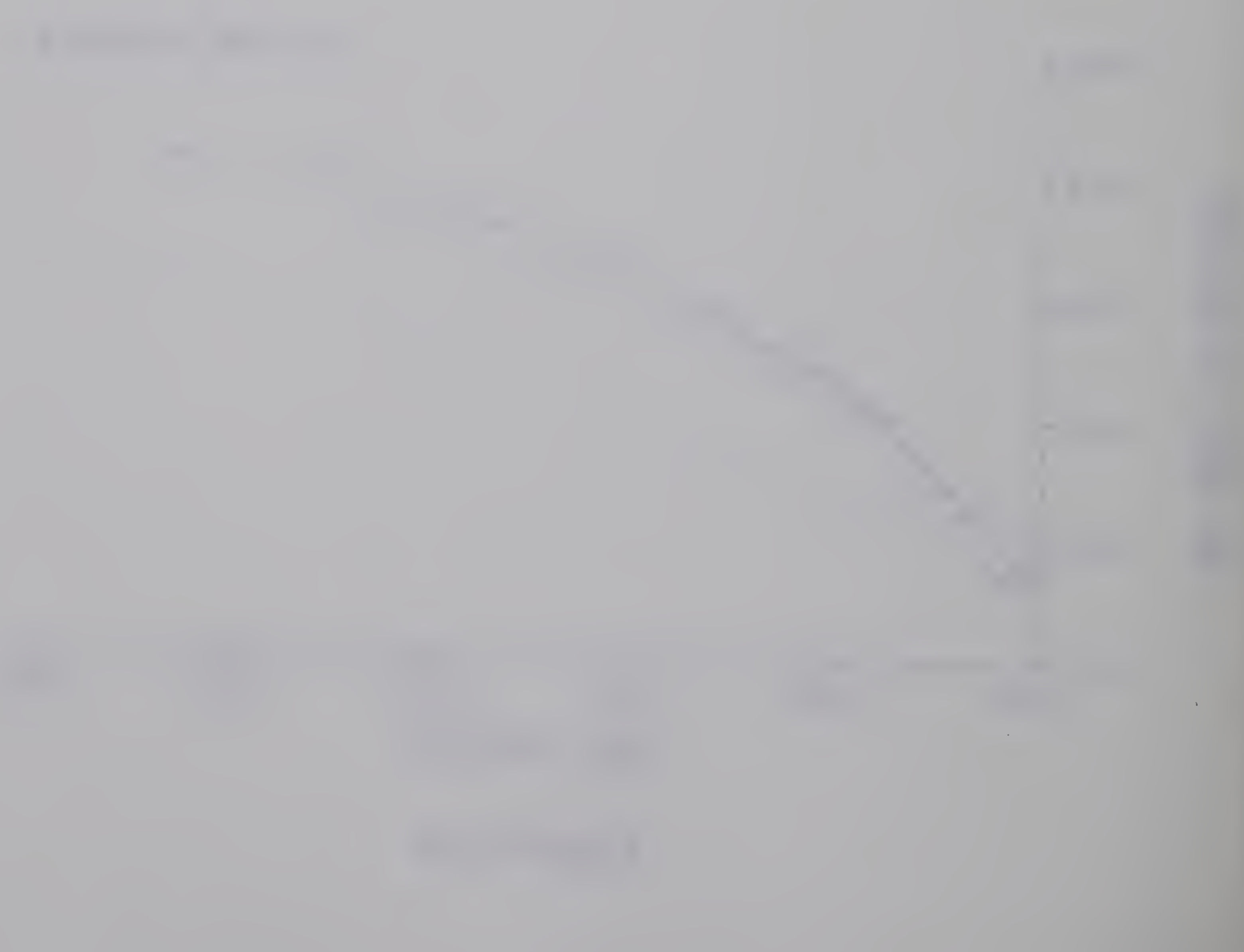

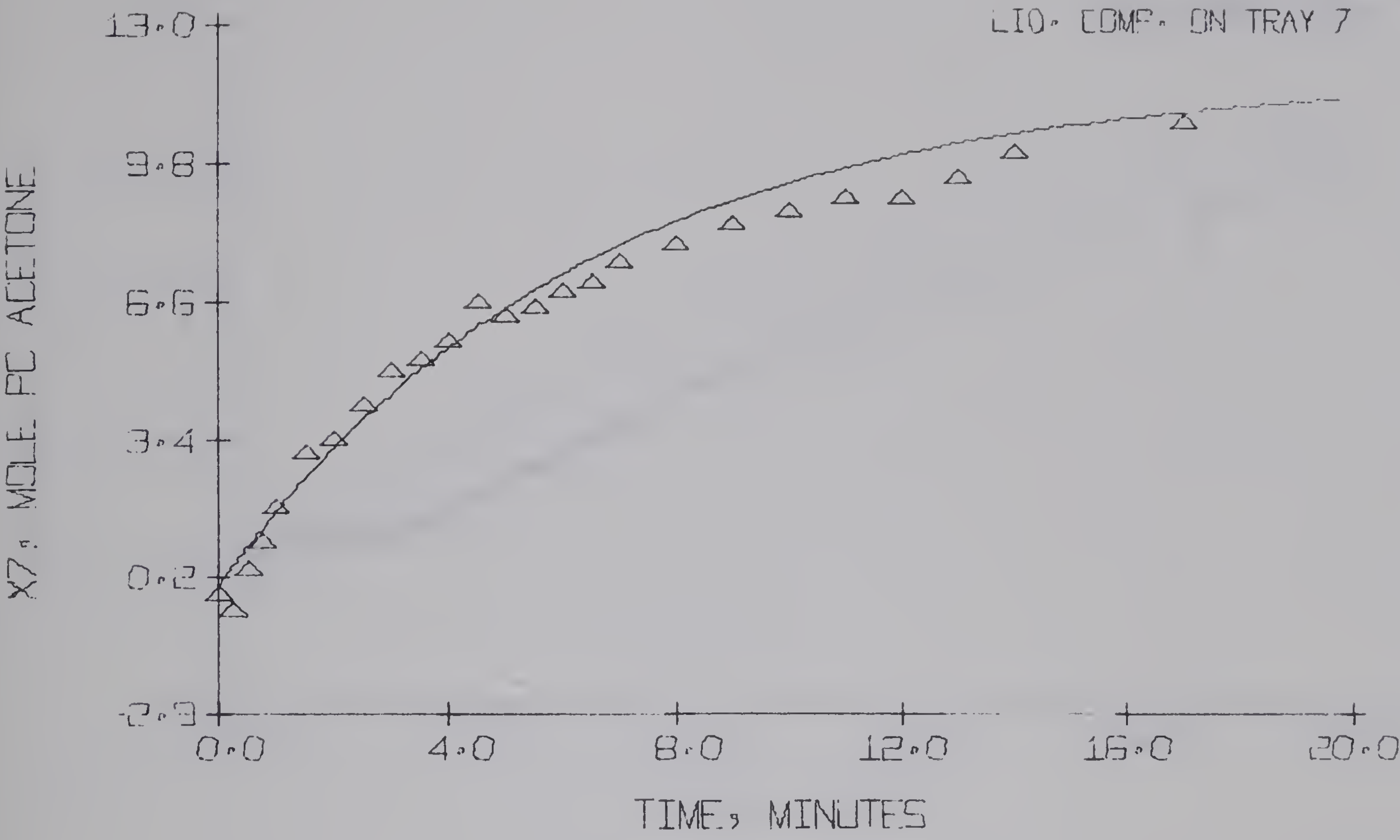

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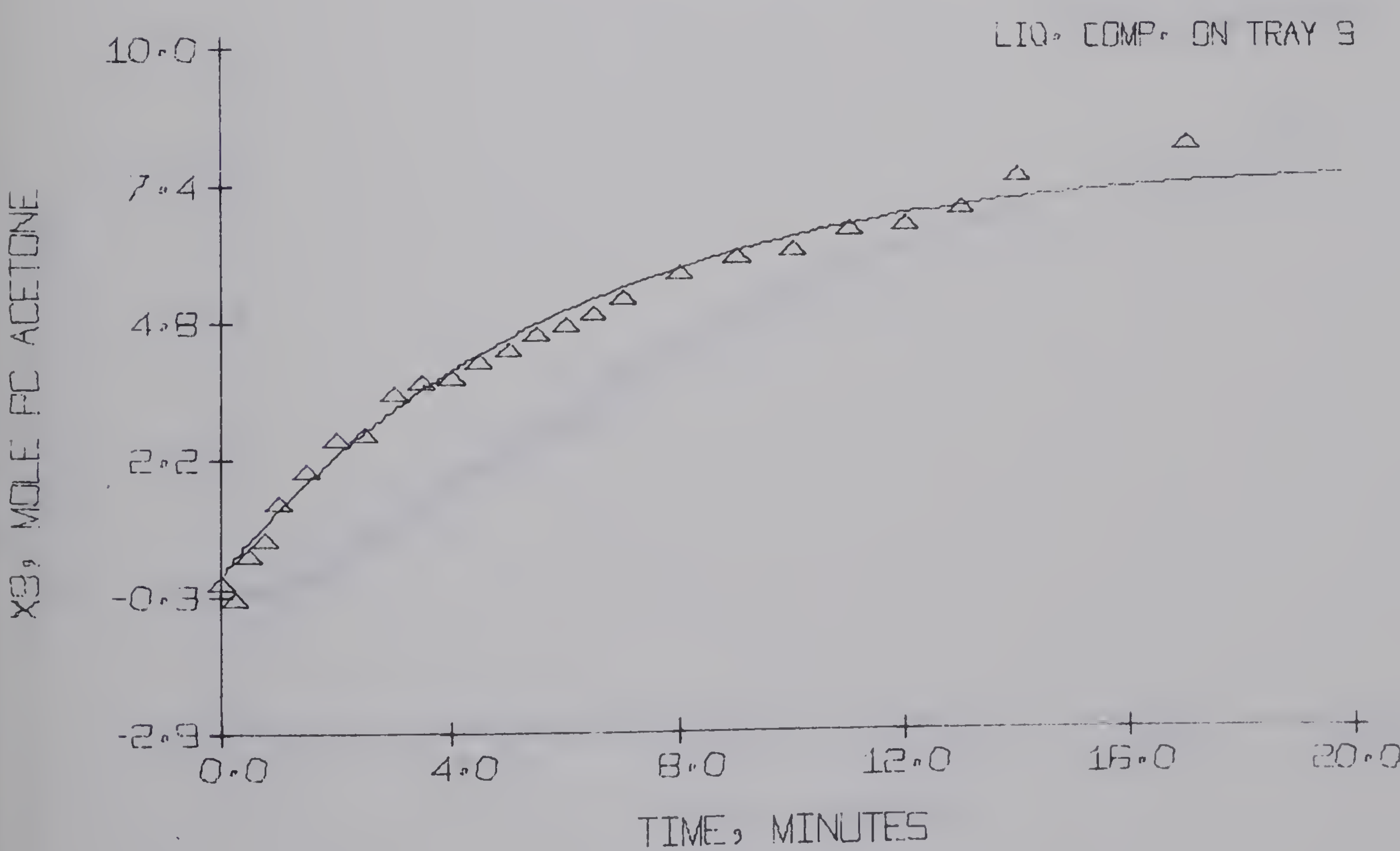

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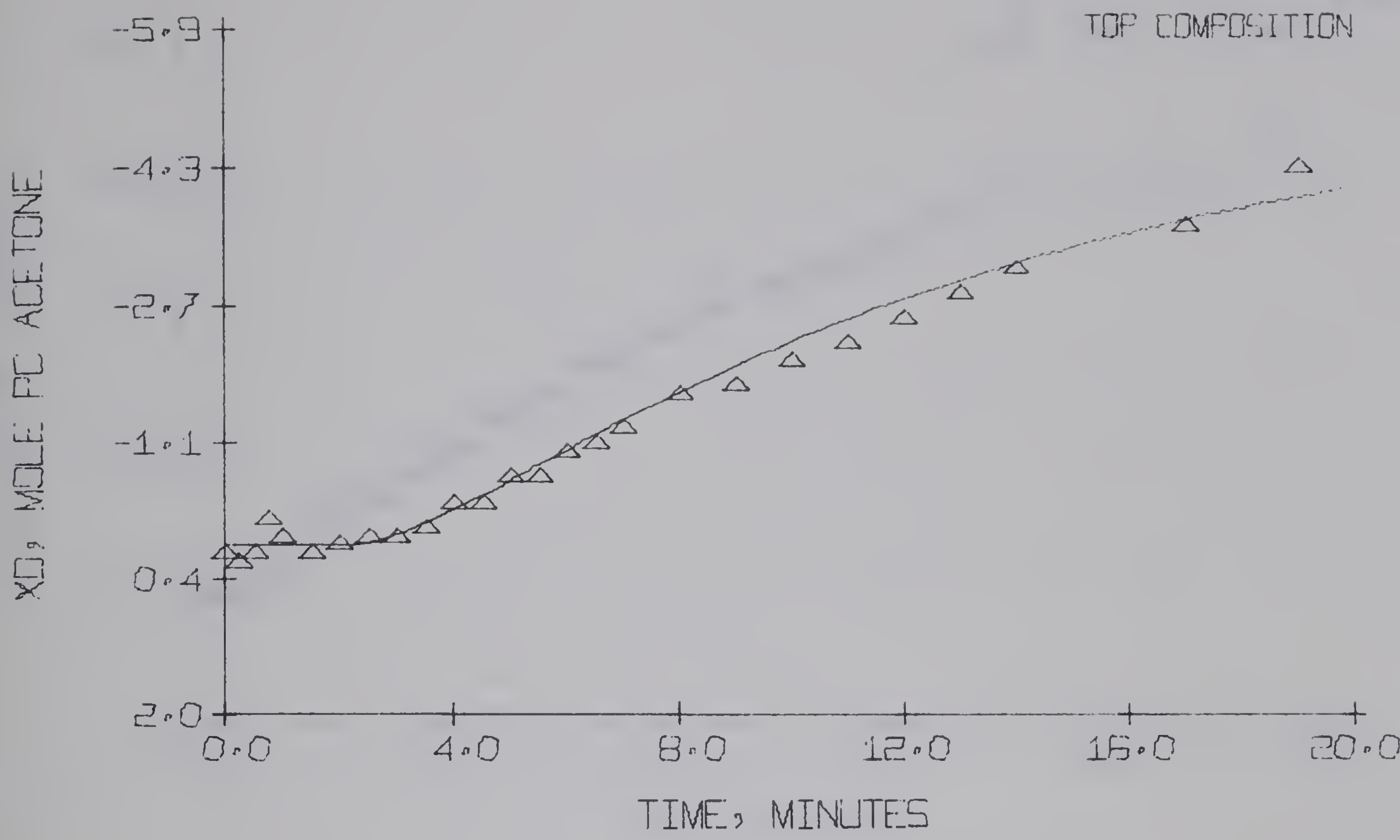

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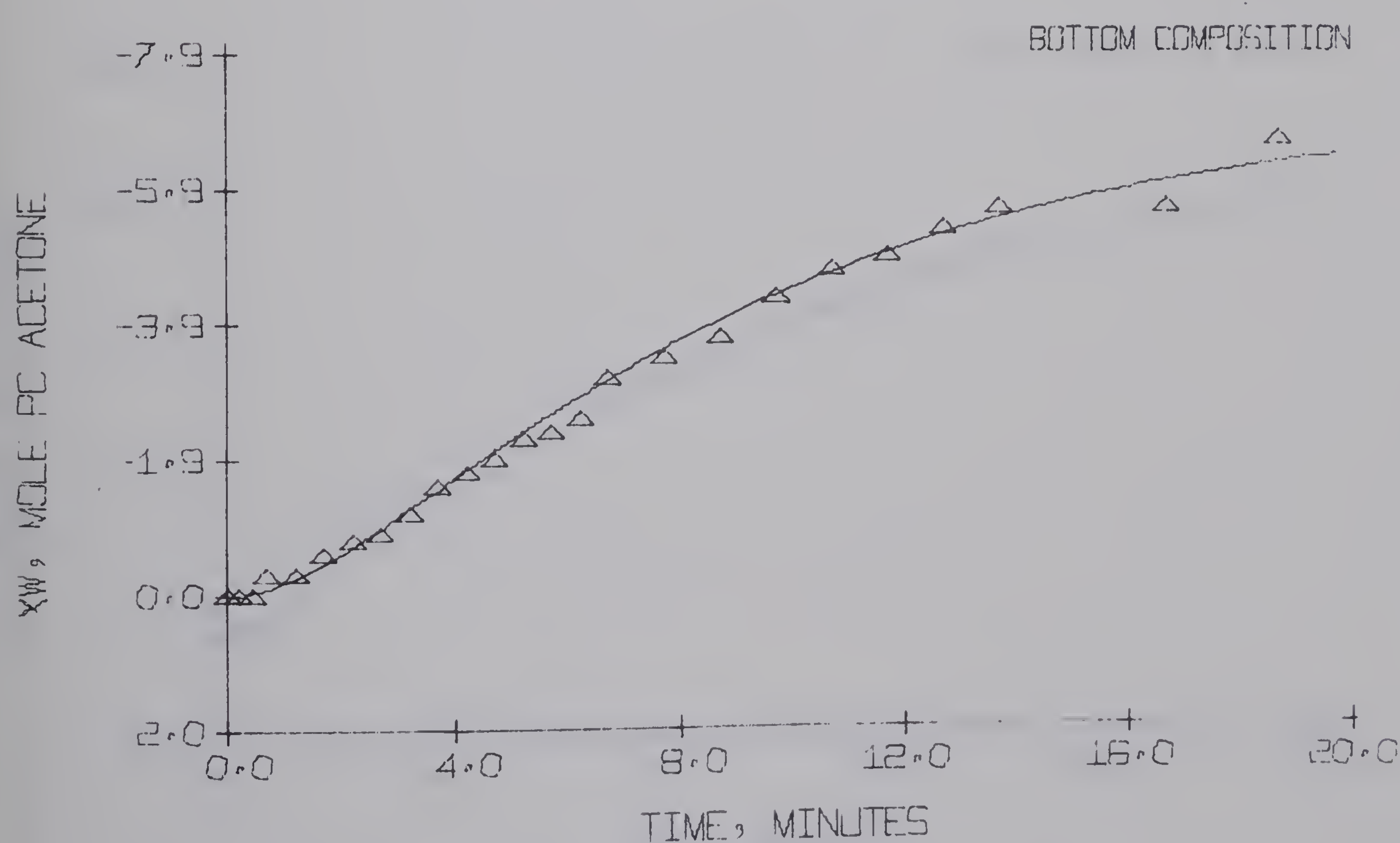

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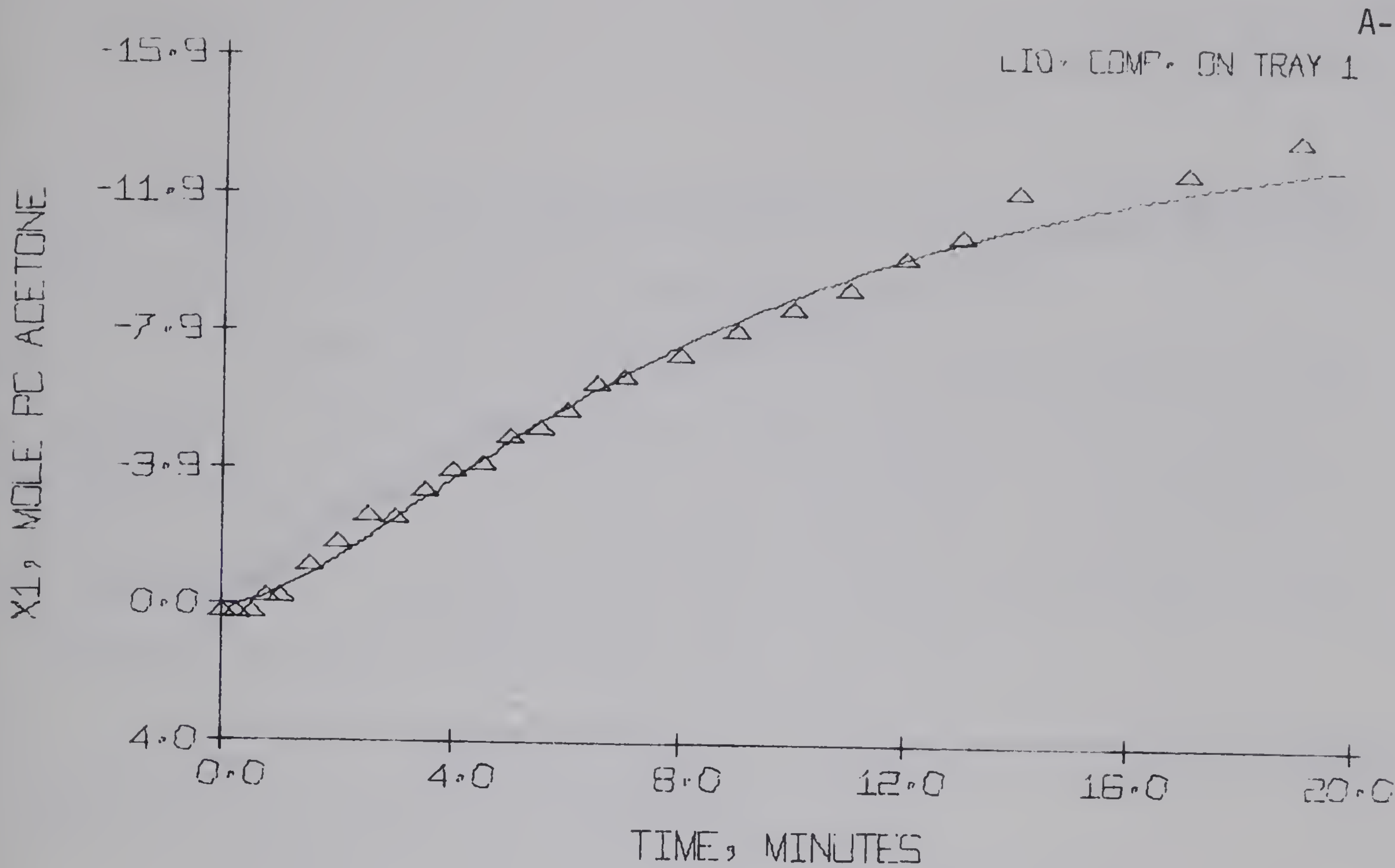

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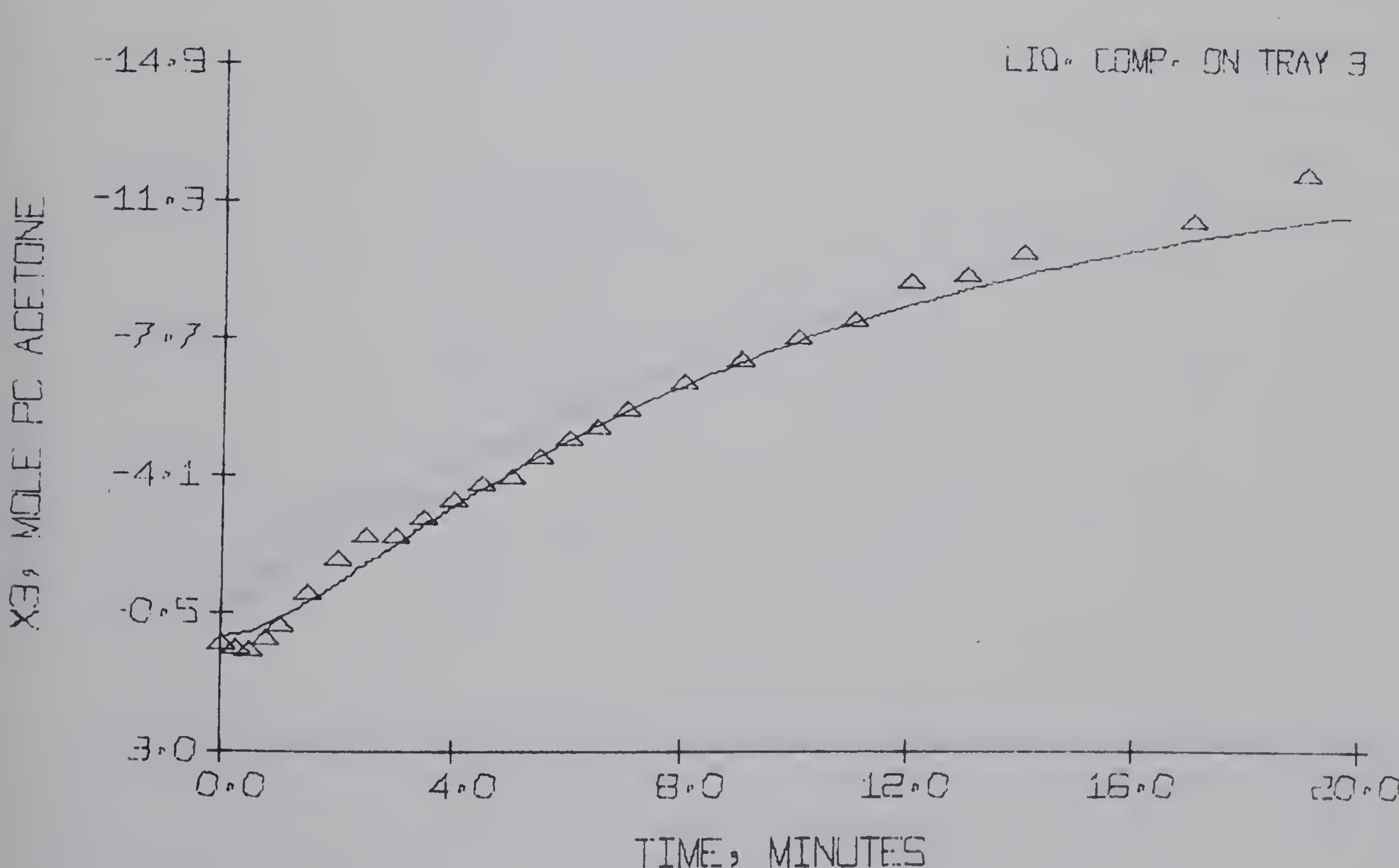

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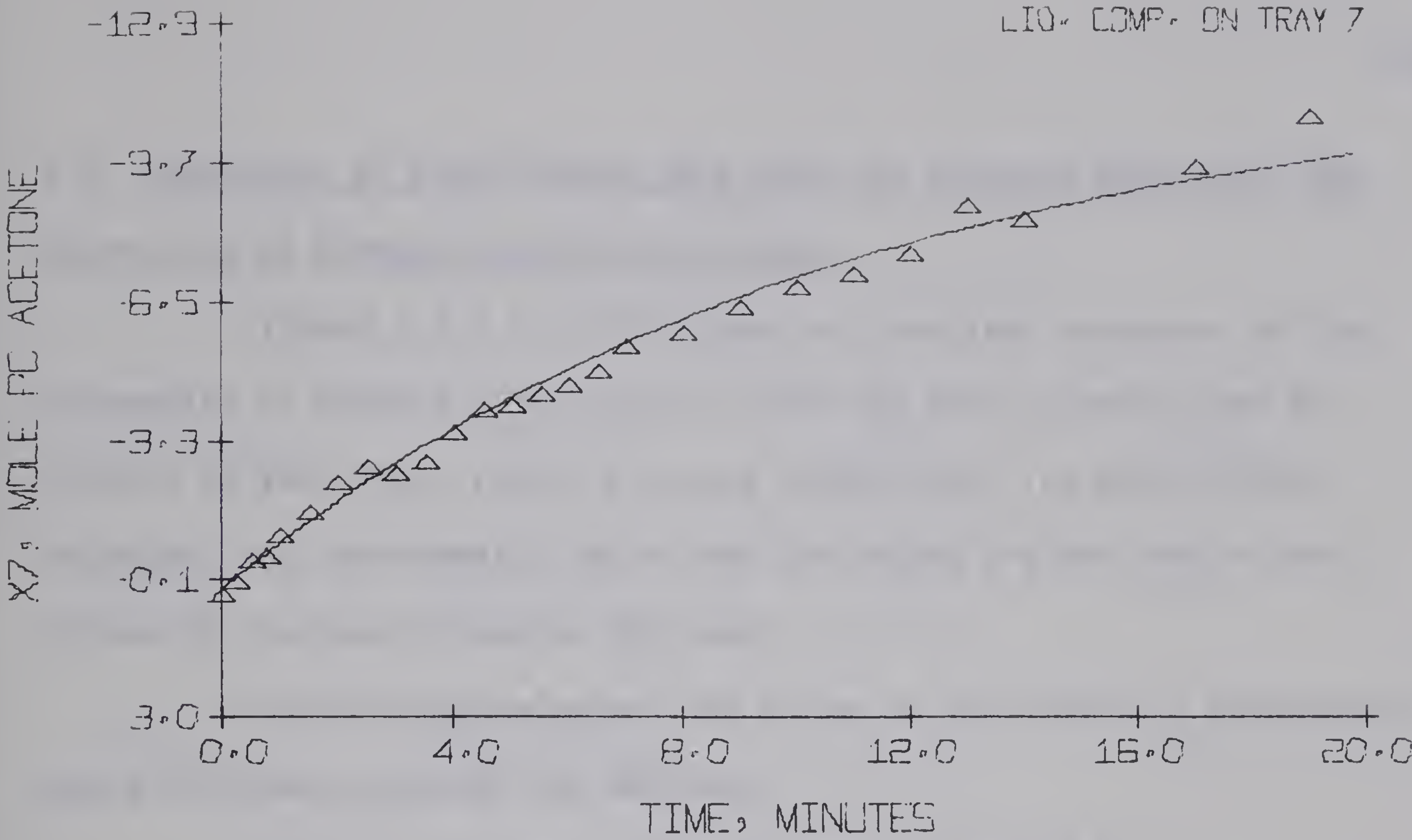

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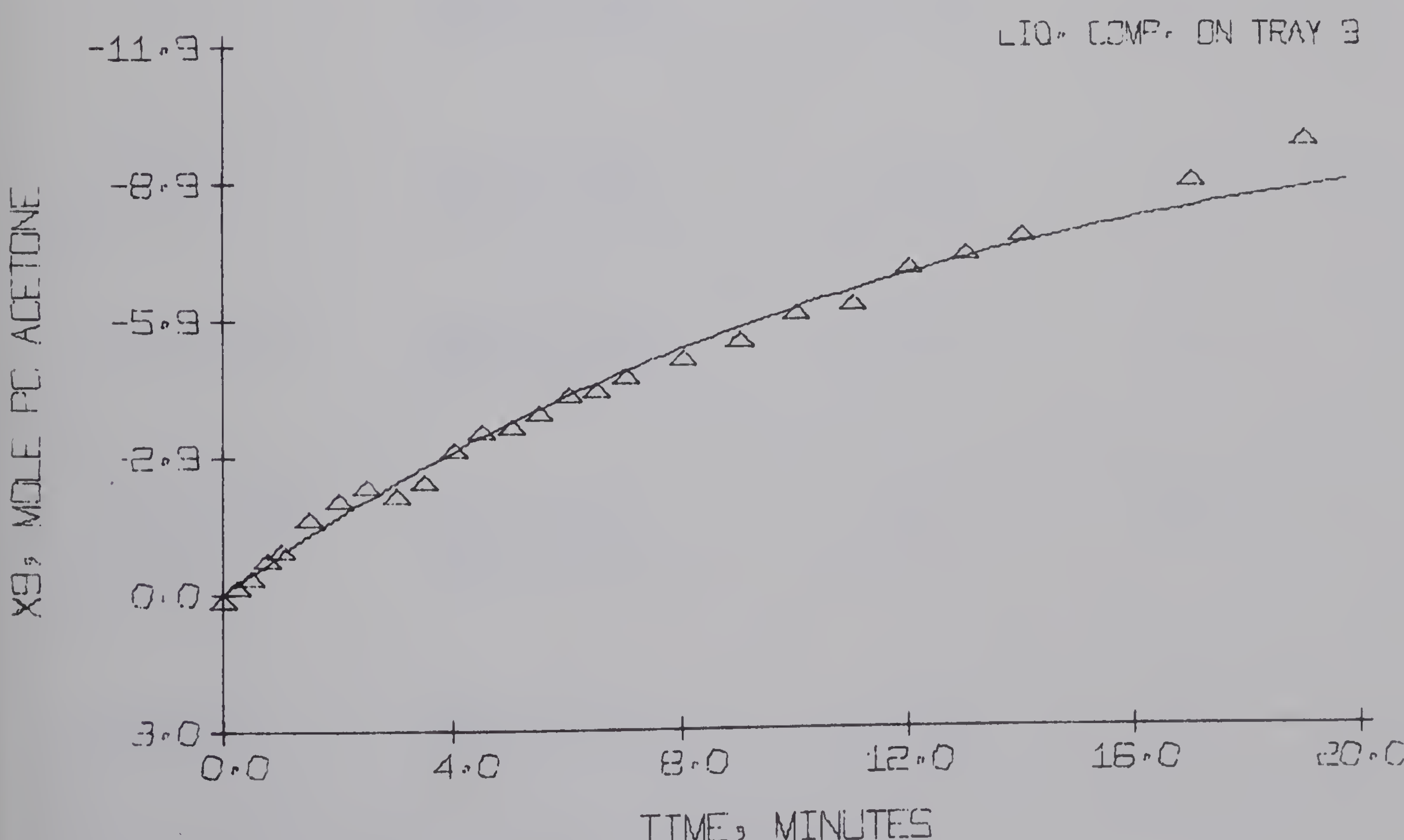


Figure A.1-18

A.2 Comparison of Experimental Data with the Proposed Models for the University of Alberta Distillation Column

Figures A.2-1 to A.2-60 show the transient responses of the University of Alberta distillation column for both increases and decreases in feed flow, reflux flow and steam flow. The solid lines represent the experimental values and the points are the data as predicted by the models used in this work.

The disturbance enters the column in the form of a rectangular pulse of known magnitude and duration.

Captions for these figures appear in Table A.2-1.

Table A.2-1

Captions for Figures A.2-1 to A.2-60

Figure Identification	Disturbance	Pulse Magnitude (lb./min.)	Pulse Duration (min.)
A.2-1 to A.2-10	Feed Flow (Run No. 24*)	2.57 to 3.02	9.6
A.2-11 to A.2-20	Feed Flow (Run No. 21*)	2.57 to 2.33	15.2
A.2-21 to A.2-30	Reflux Flow (Run No. 22*)	1.93 to 2.23	13.1
A.2-32	Reflux Flow (Run No. 21*)	1.93 to 1.75	18.4
A.2-31 and A.2-33 to A.2-40	Reflux Flow (Run No. 24*)	1.93 to 1.74	7.5
A.2-42 and A.2-49	Steam Flow (Run No. 23*)	2.01 to 2.19	8.5
A.2-41 and A.2-50 and A.2-43 to A.2-48	Steam Flow (Run No. 25*)	2.01 to 2.21	8.8
A.2-50 to A.2-60	Steam Flow (Run No. 27*)	2.01 to 1.72	5.6

*Run designation used by Berry and Pacey (13).

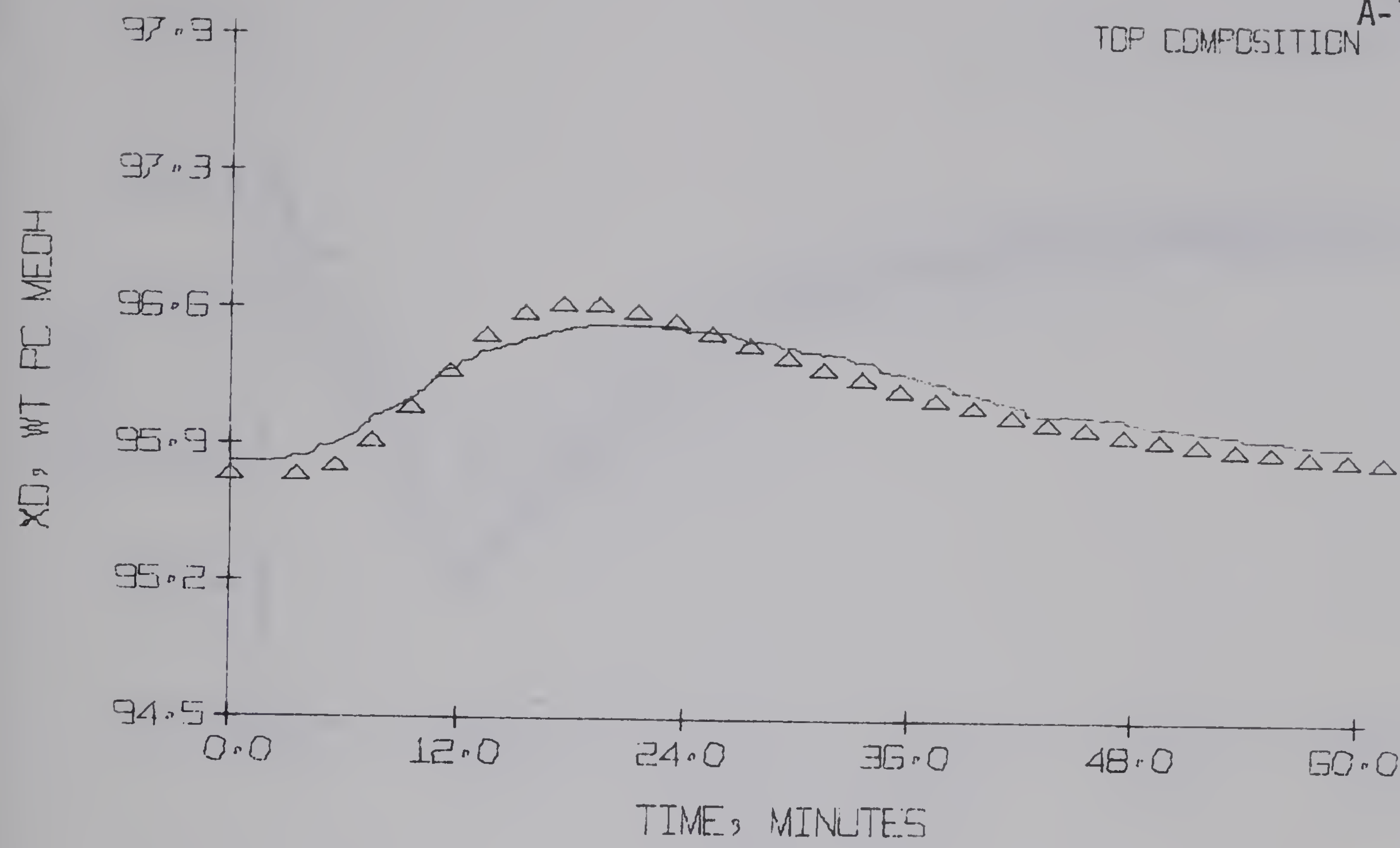
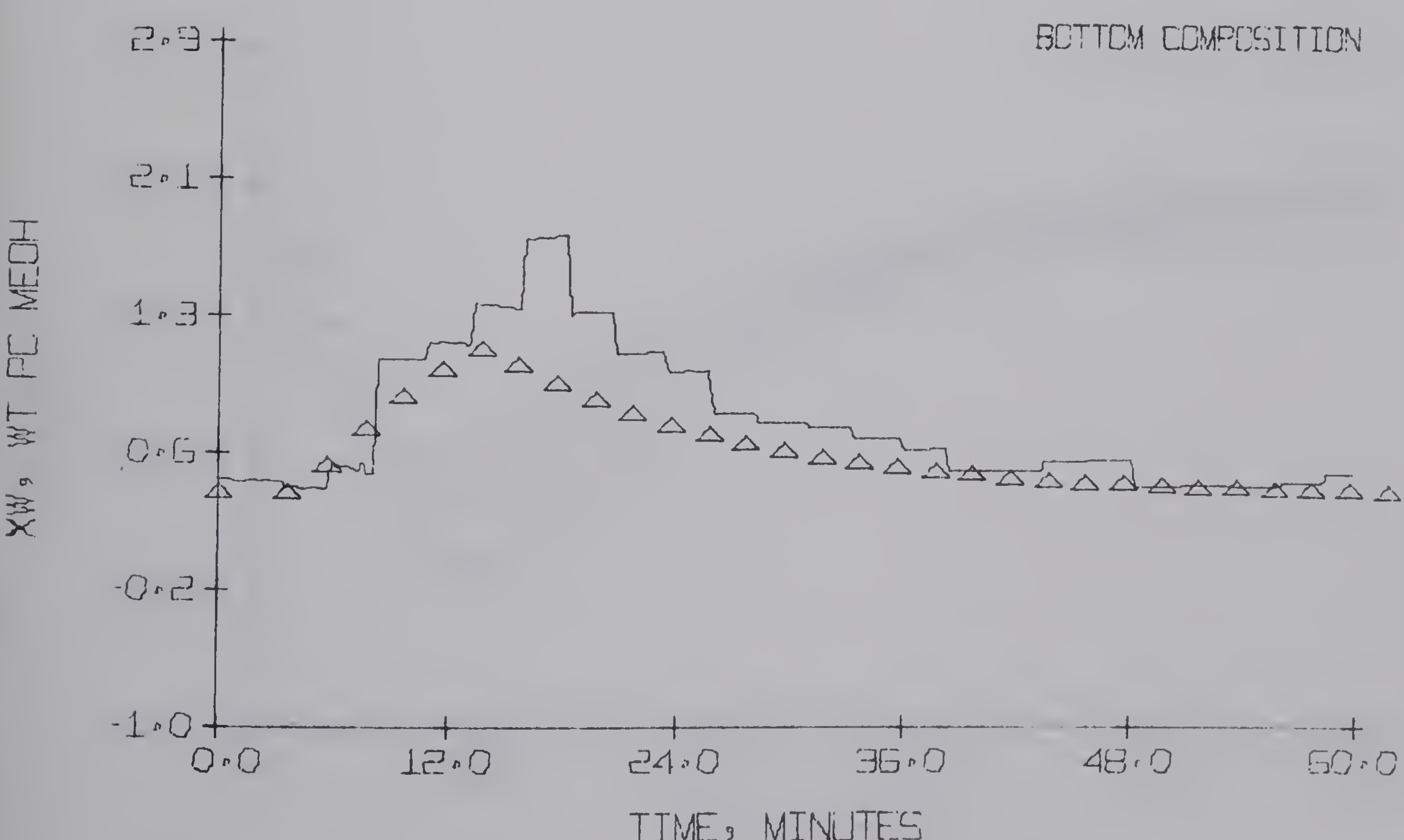


Figure A.2-1



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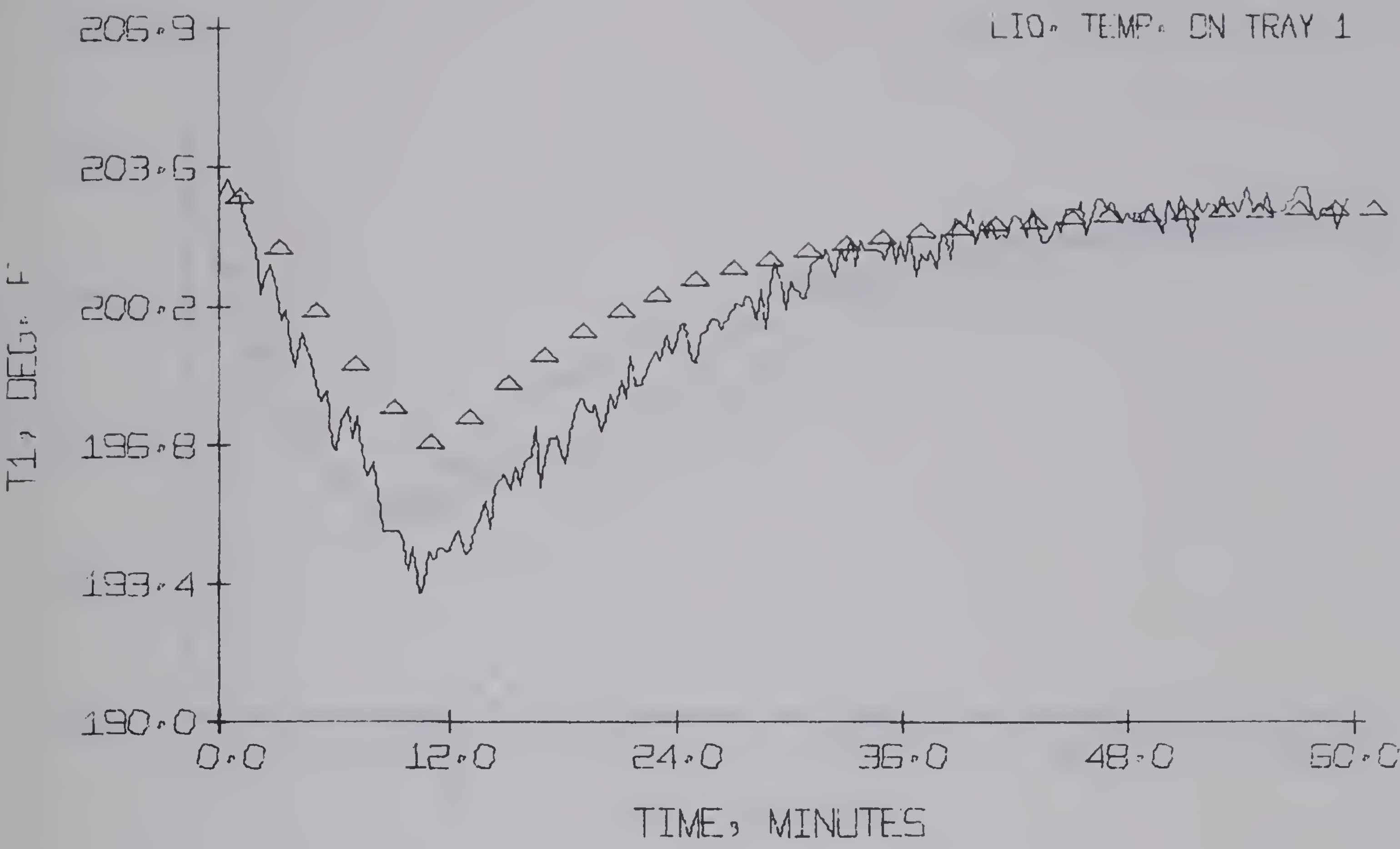

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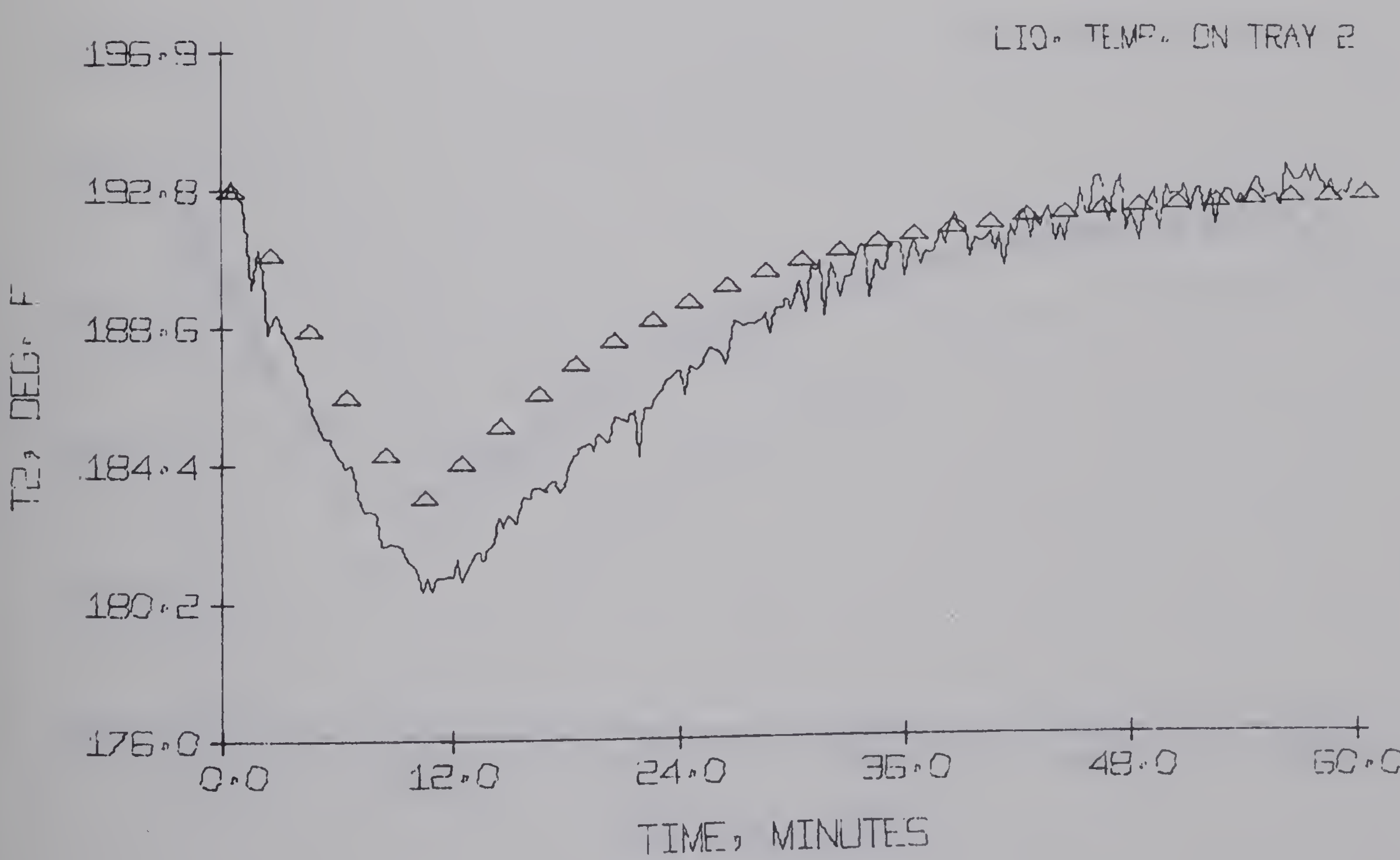

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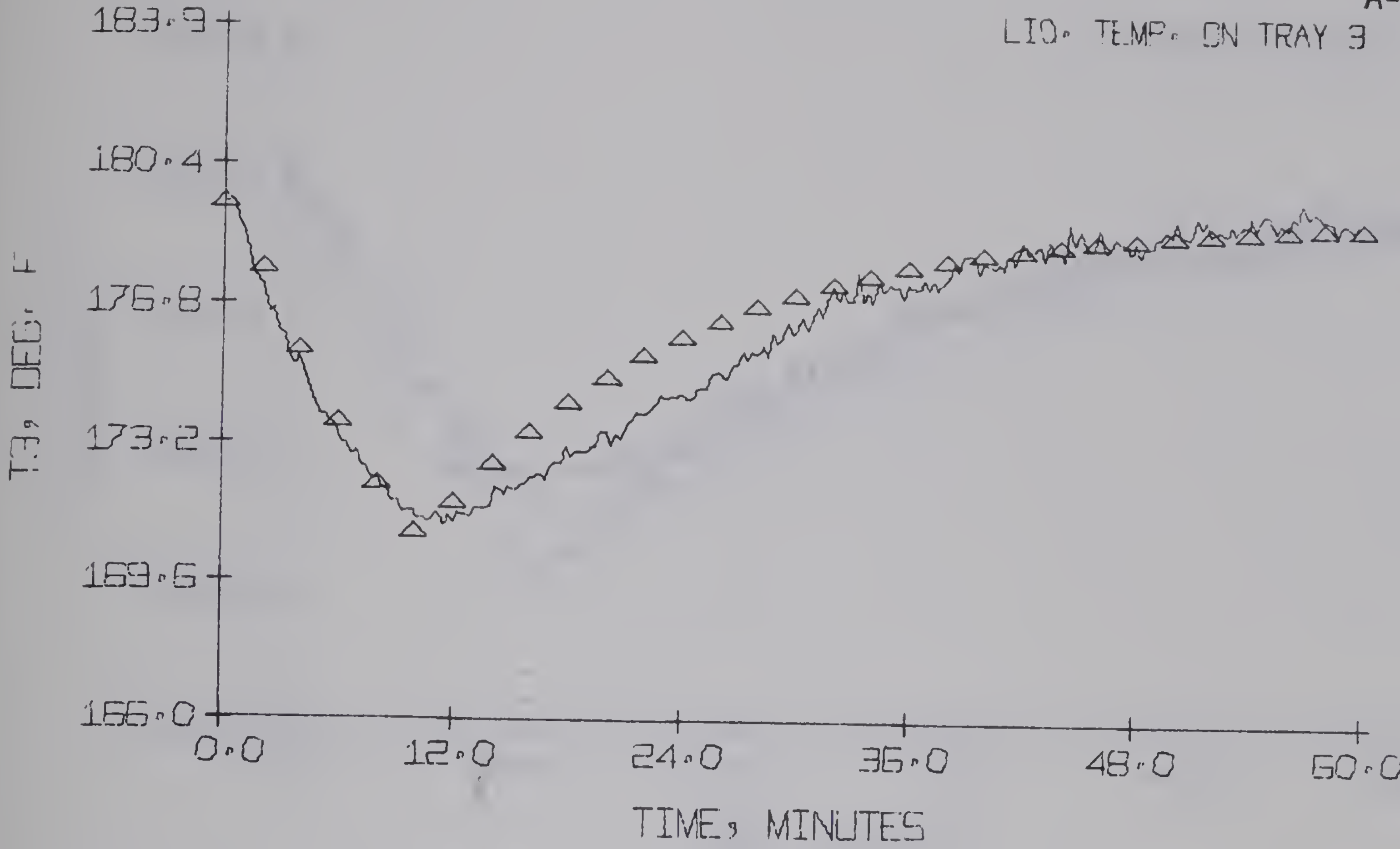

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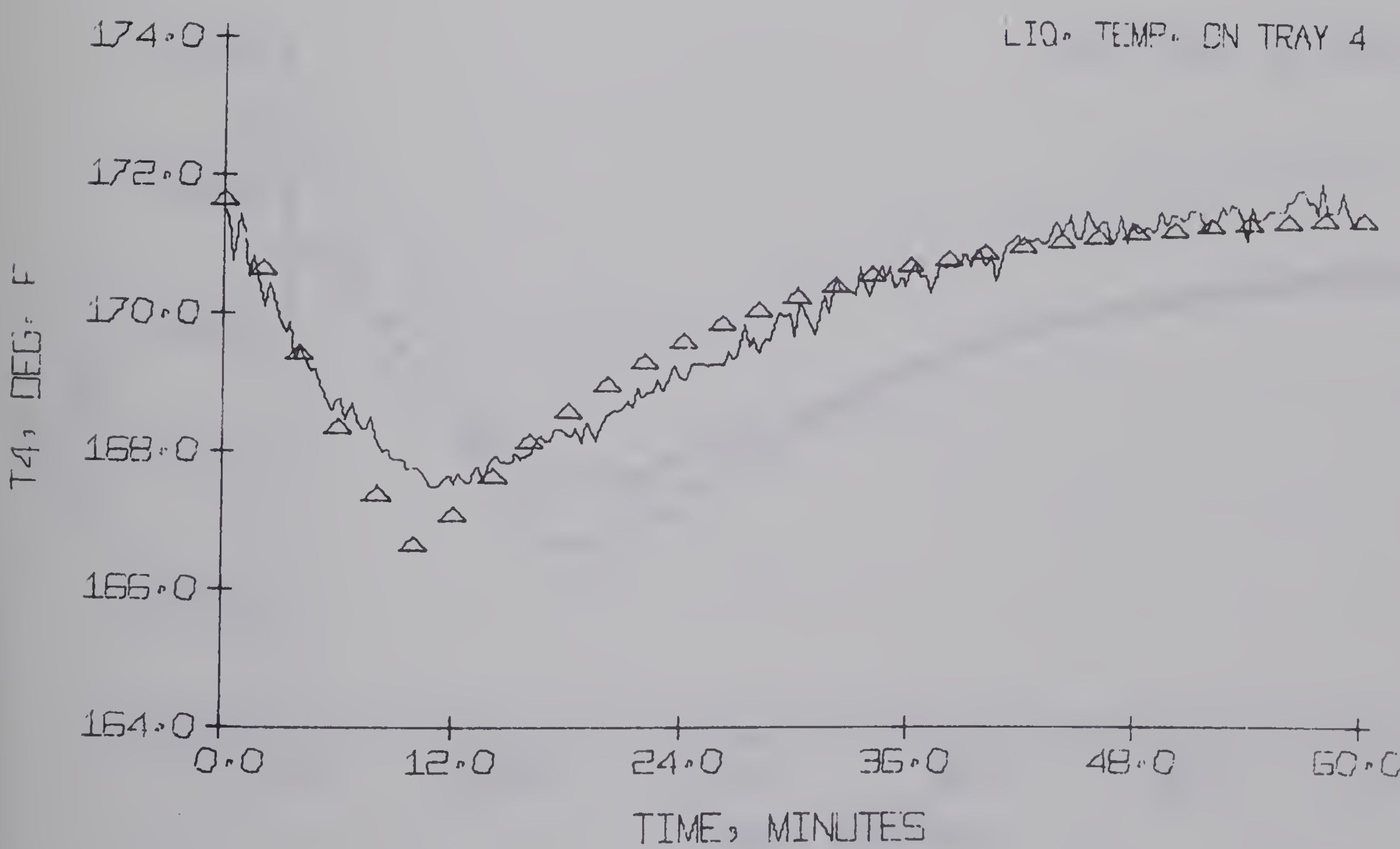

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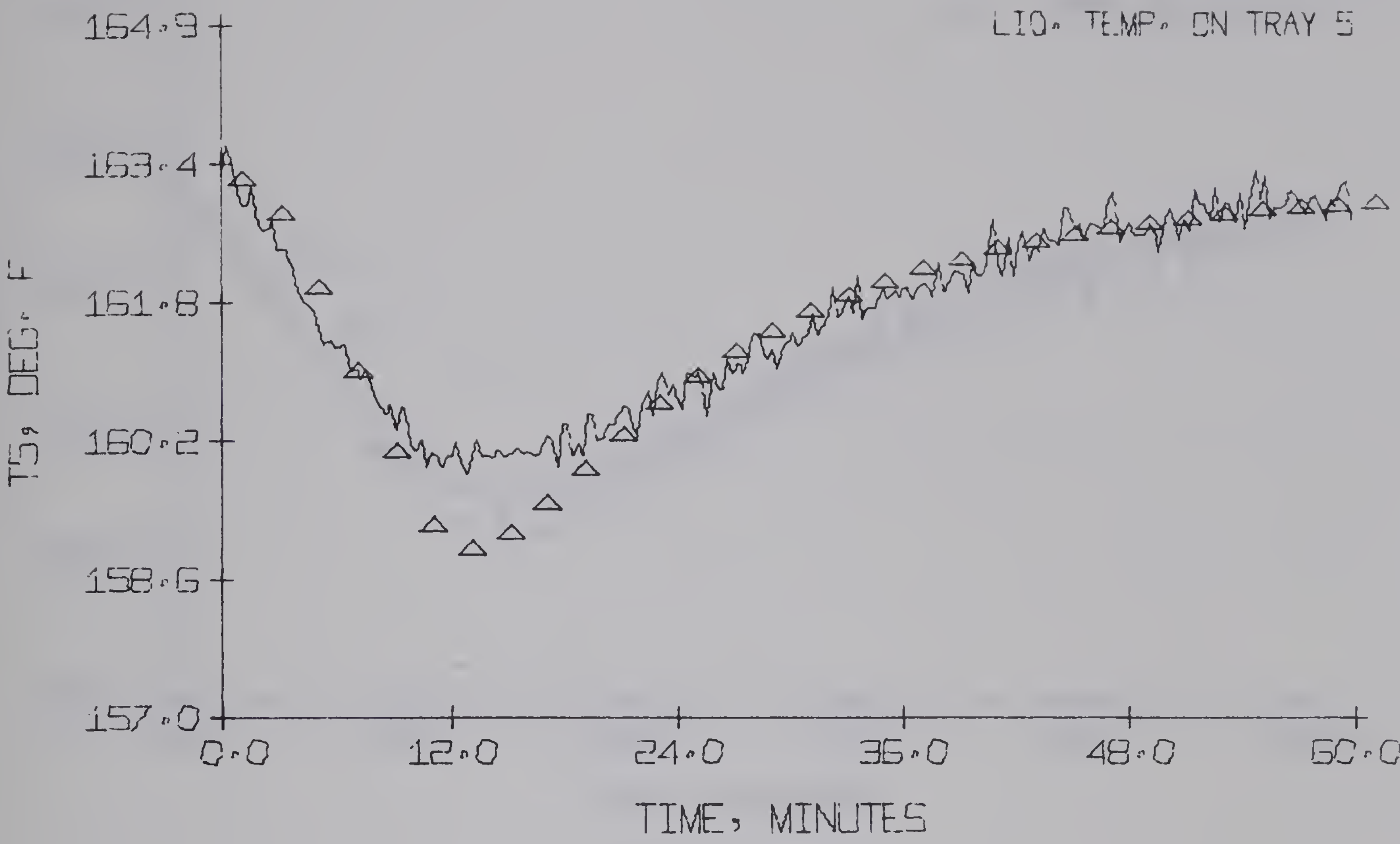

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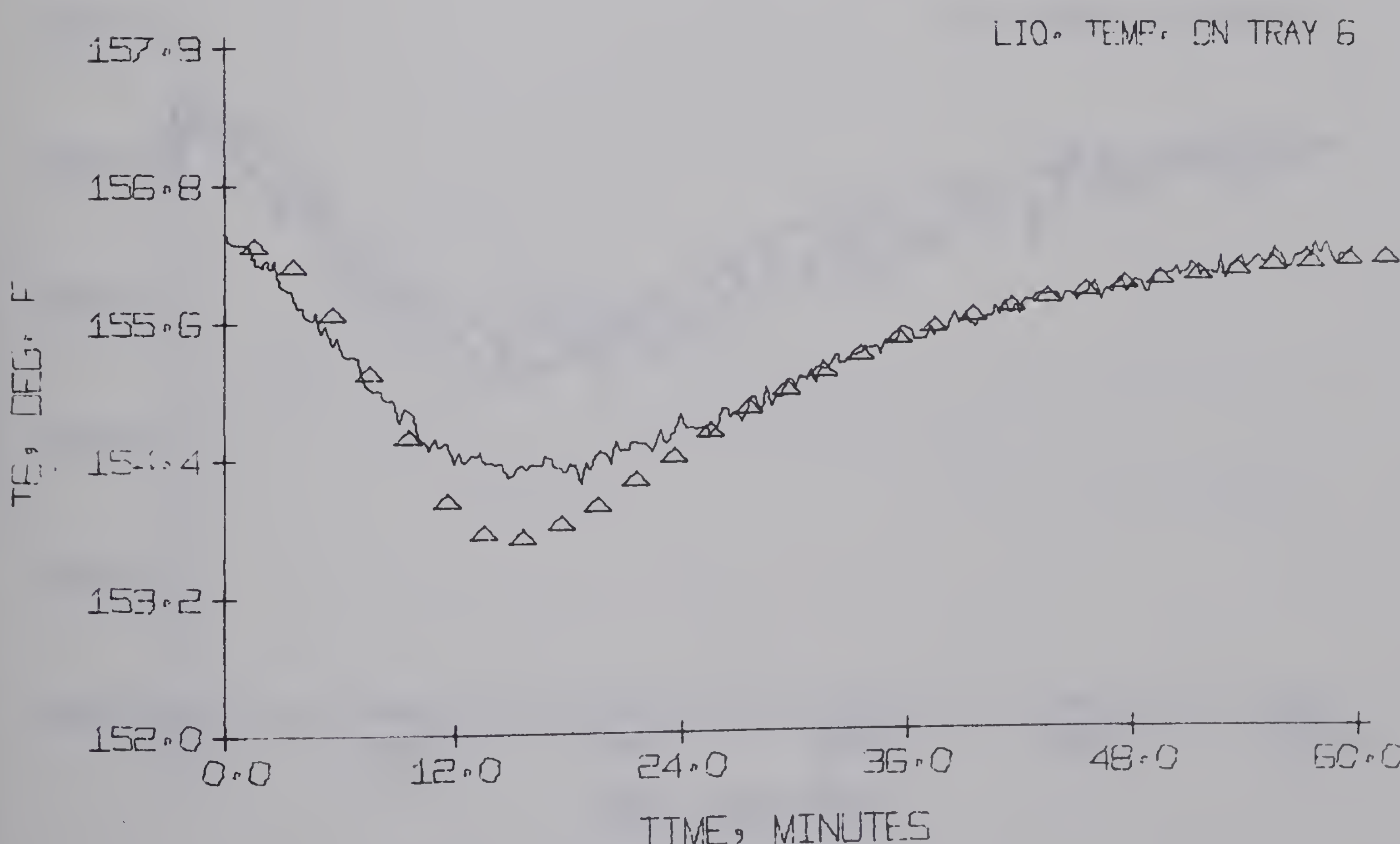

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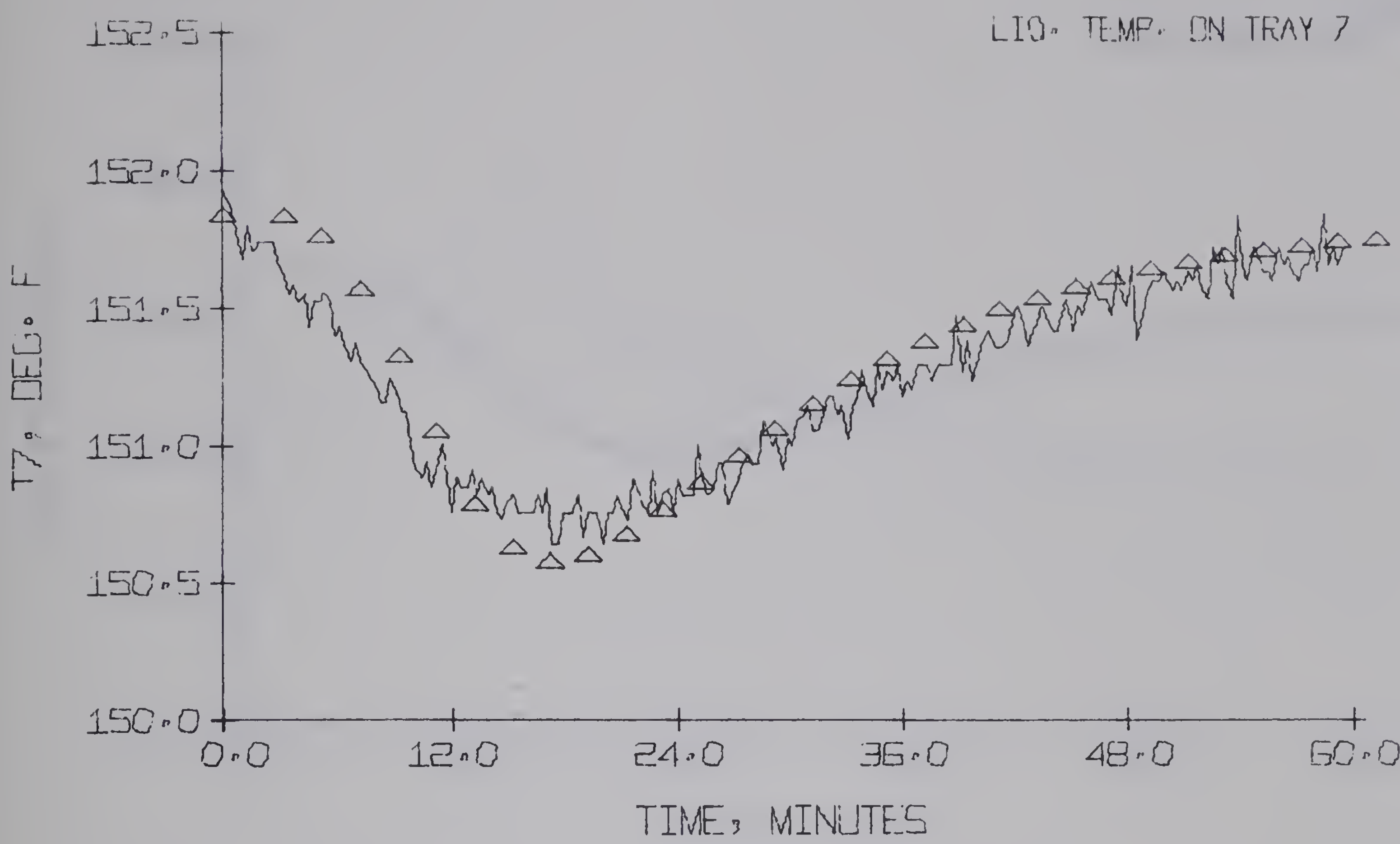

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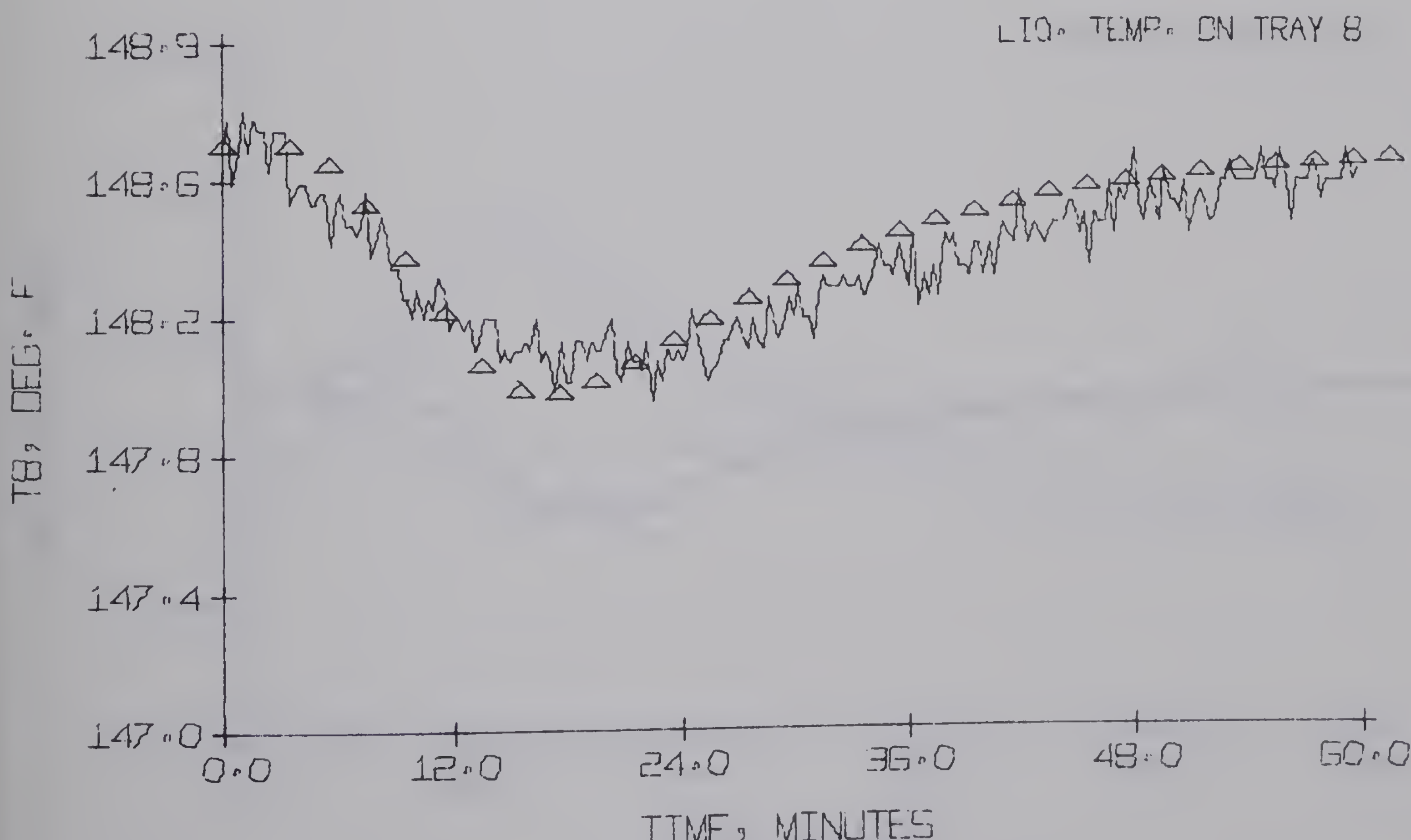

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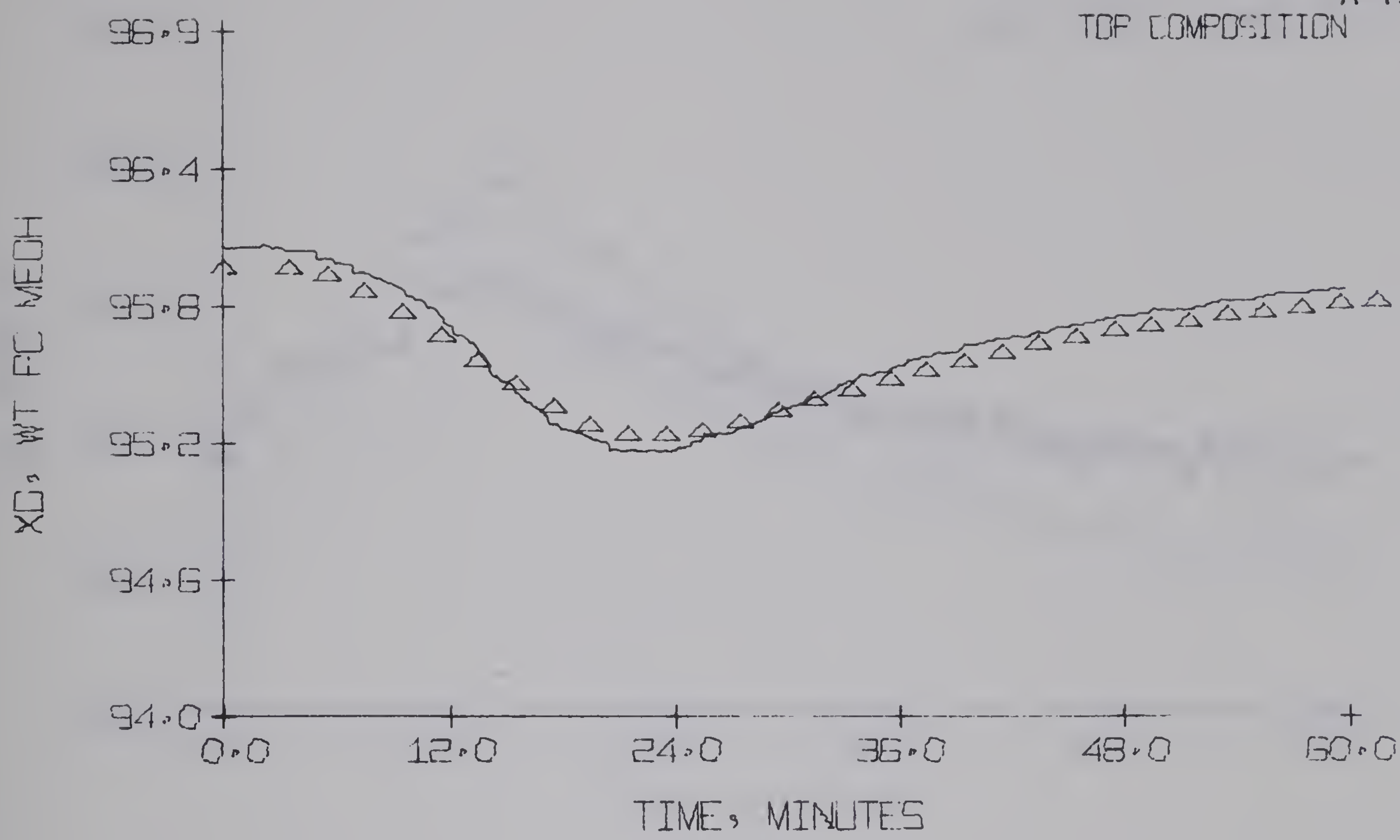

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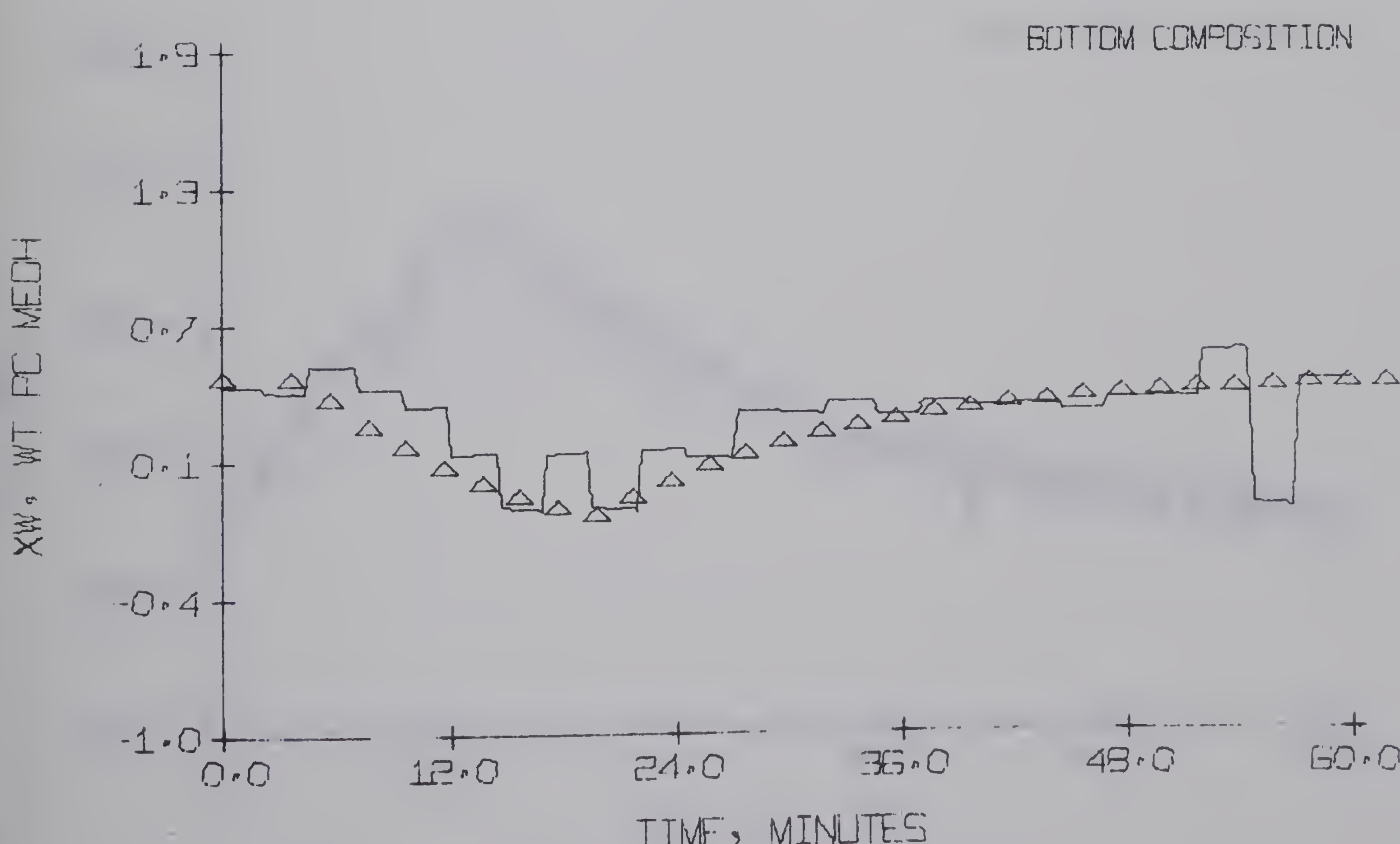

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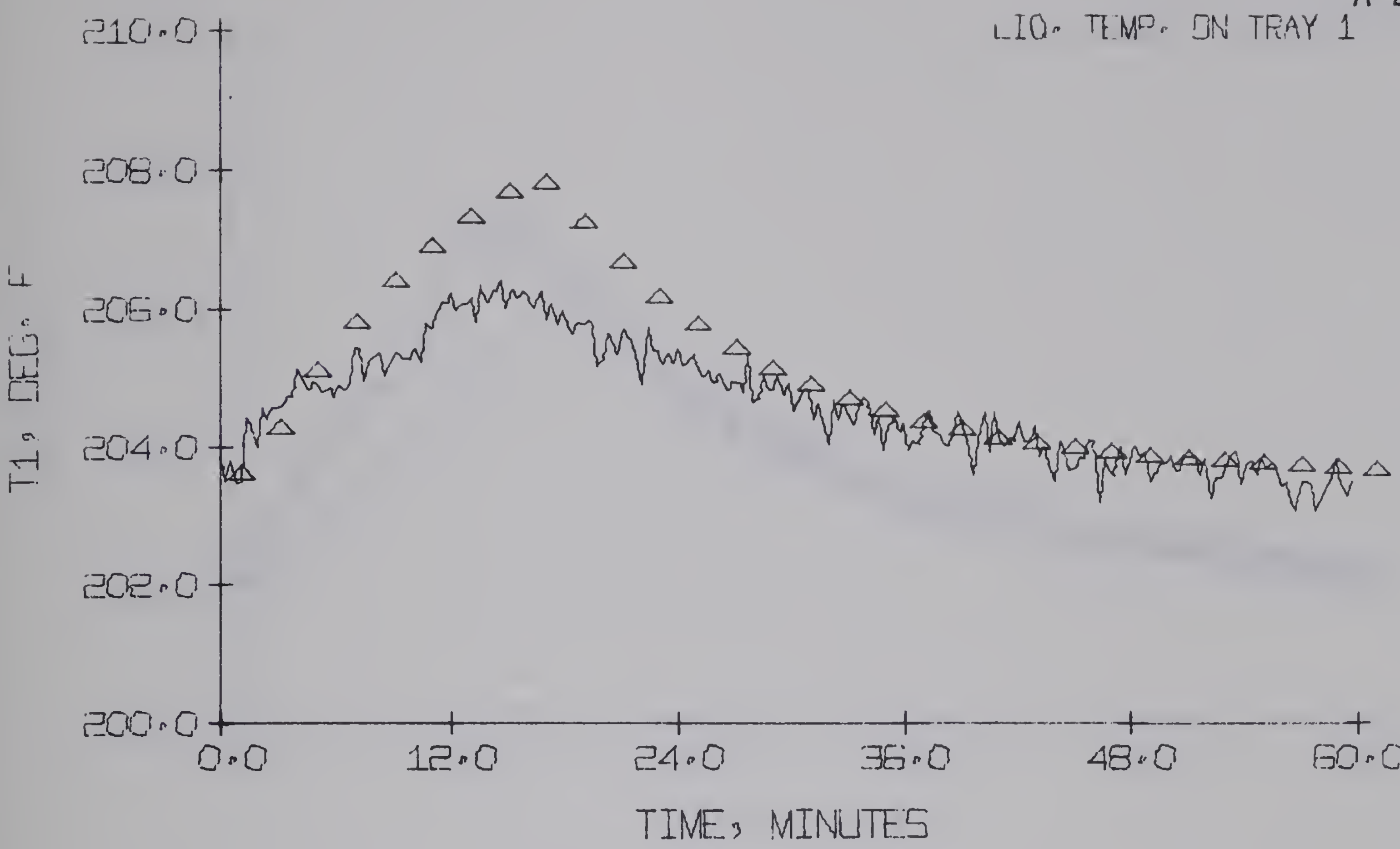

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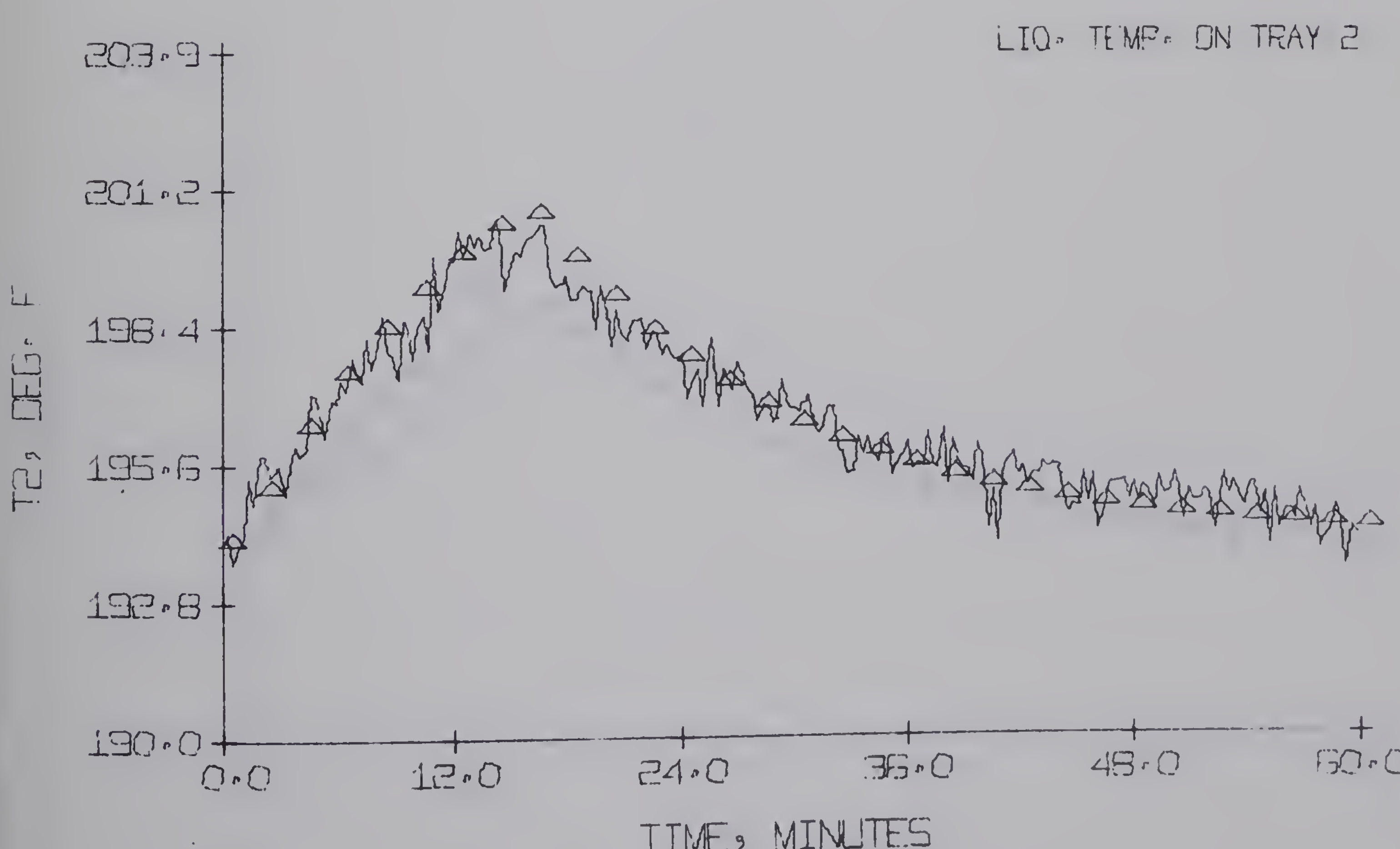

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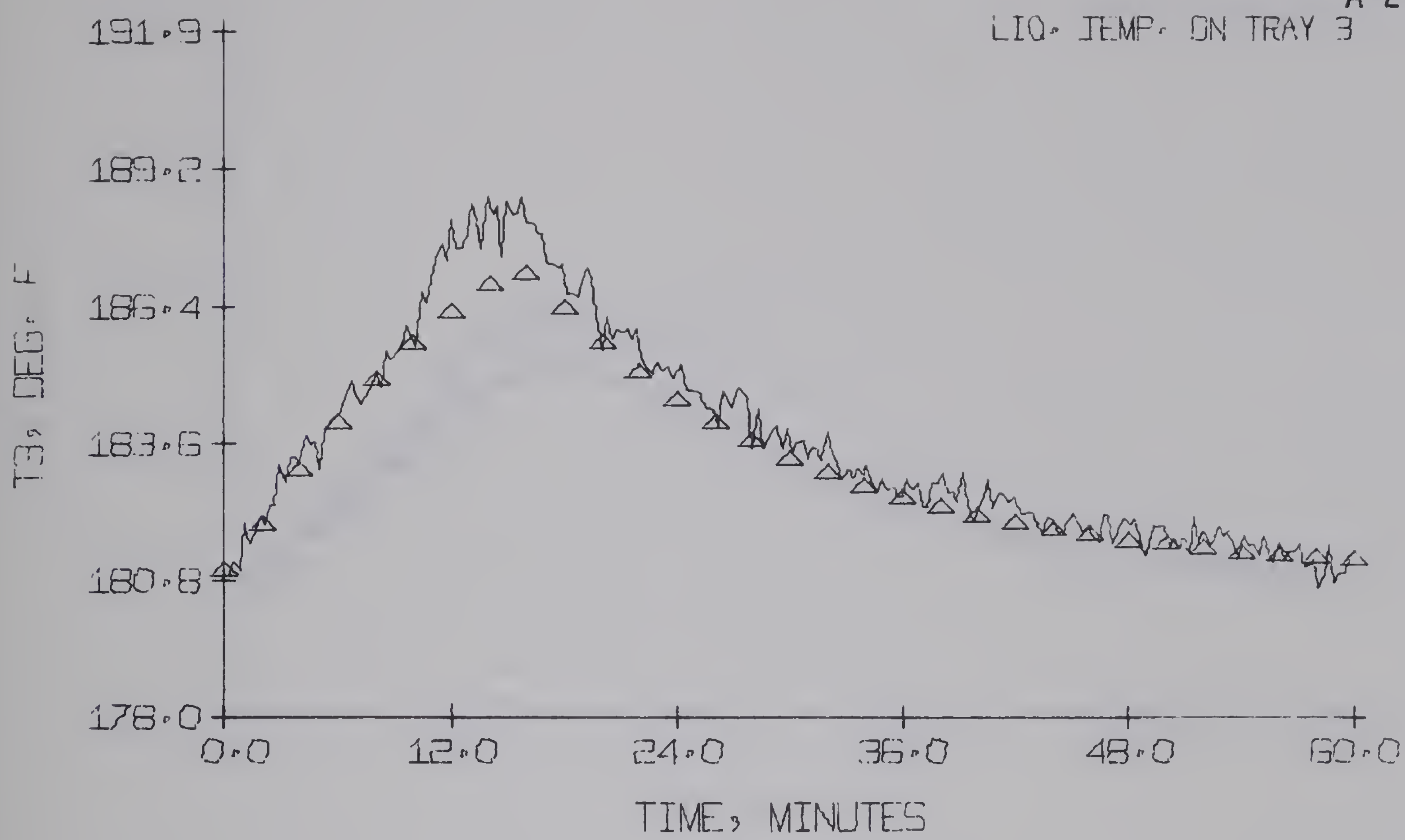

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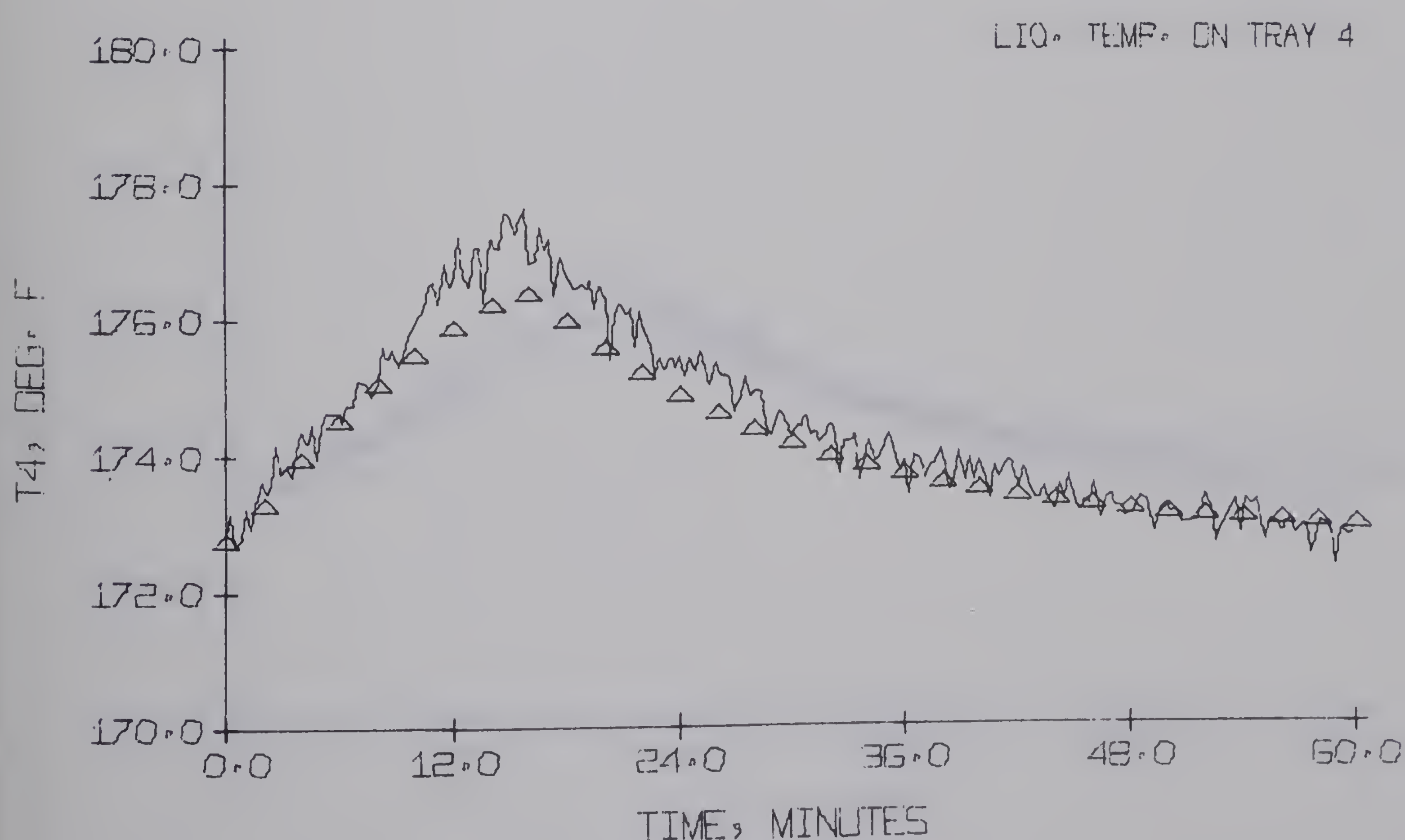

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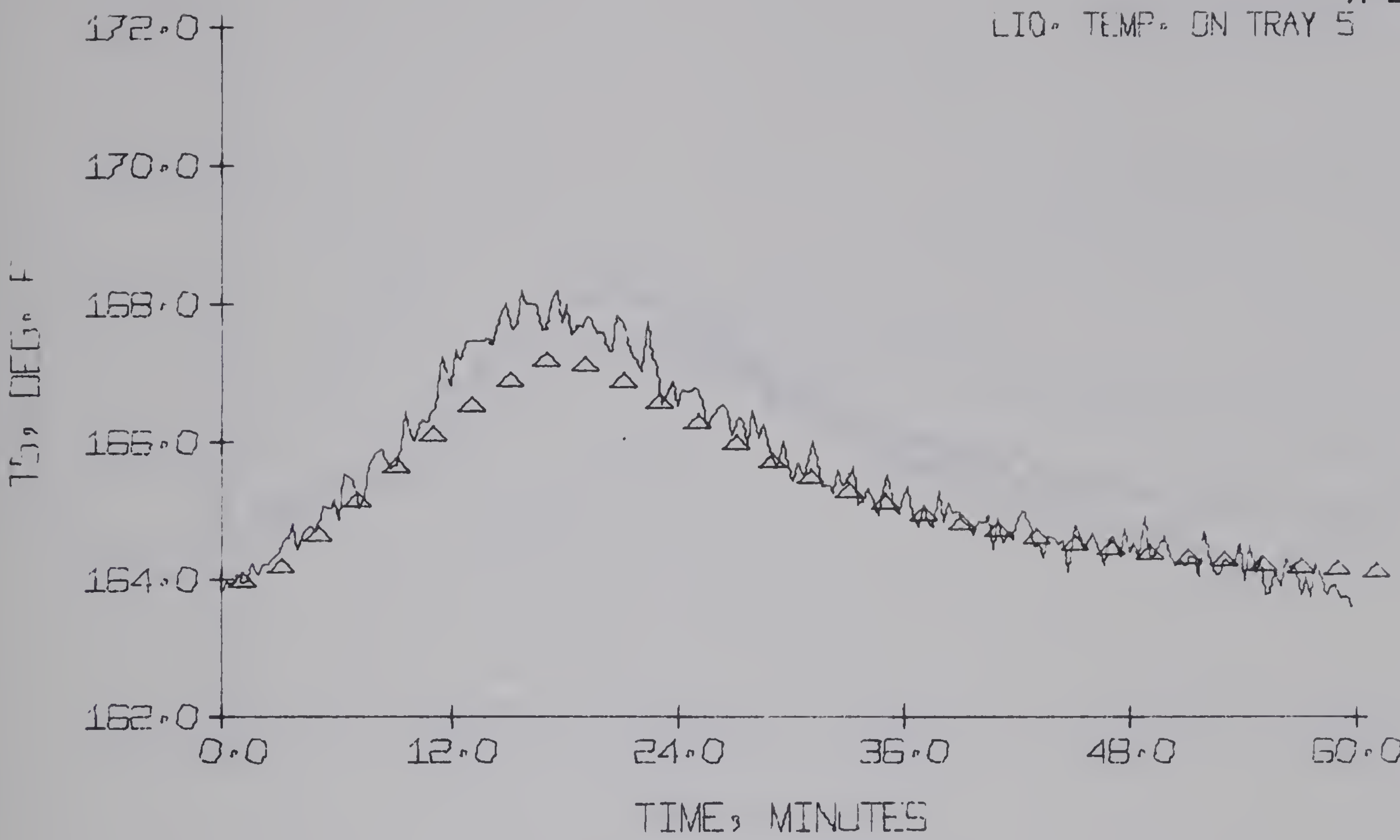

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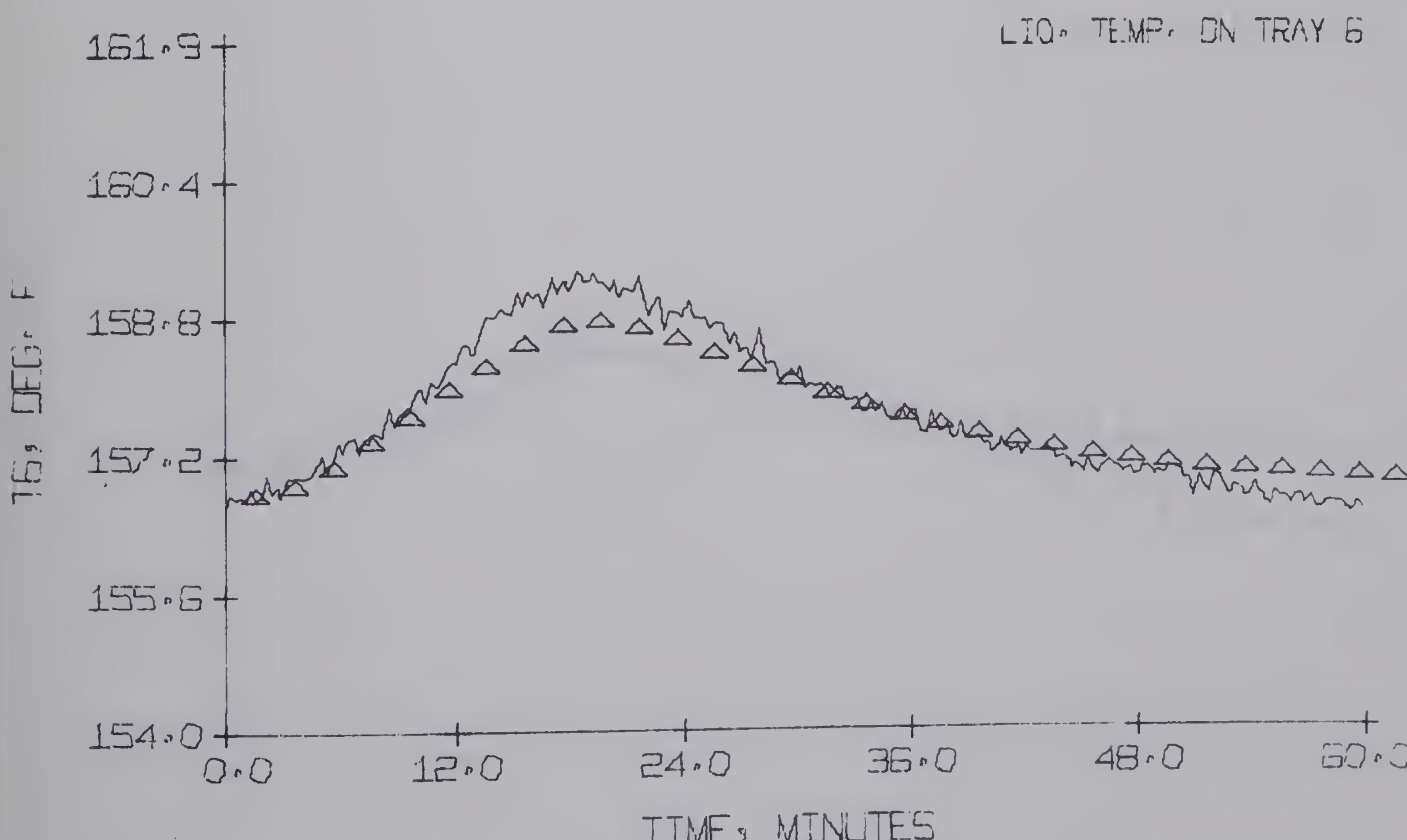

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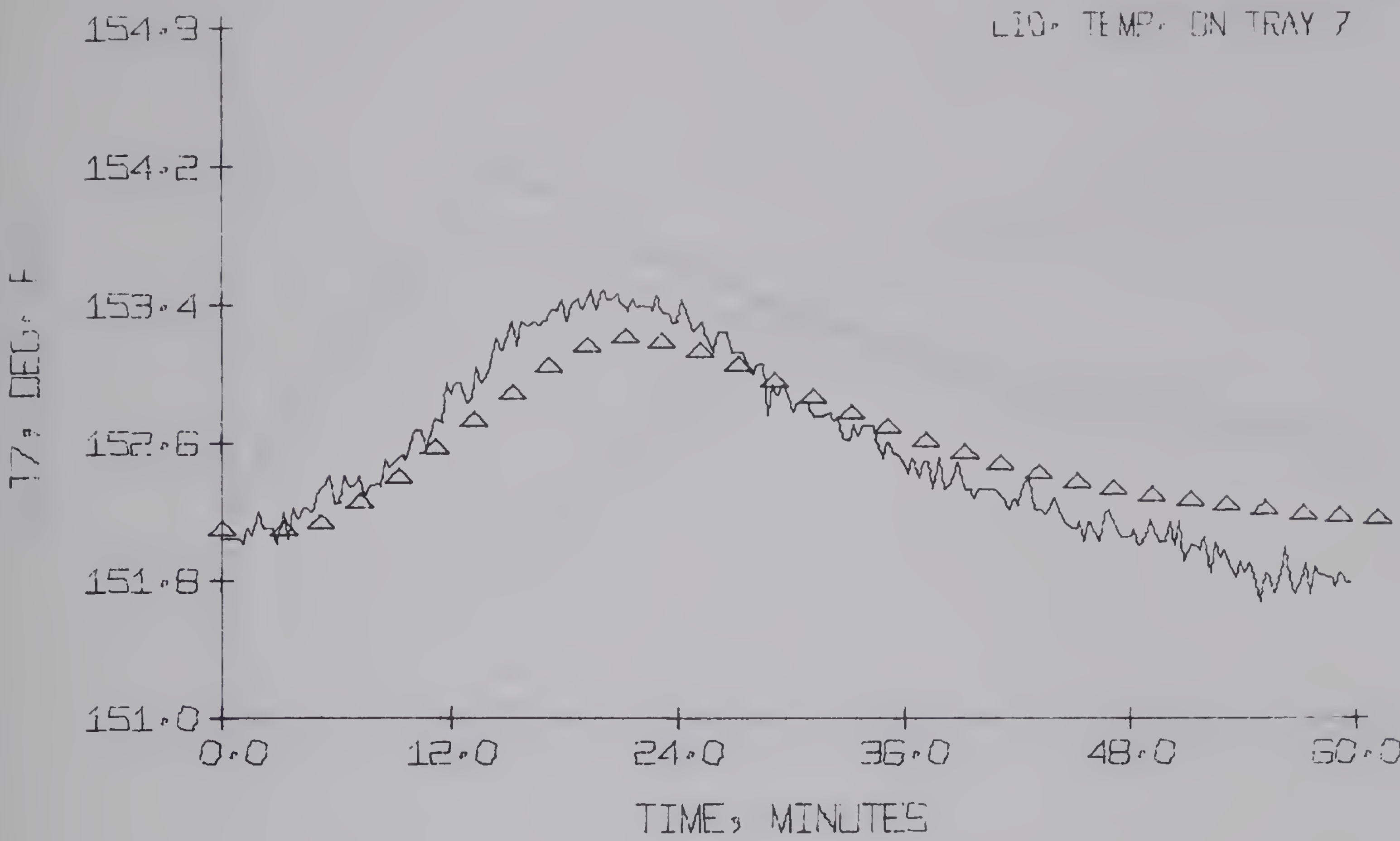

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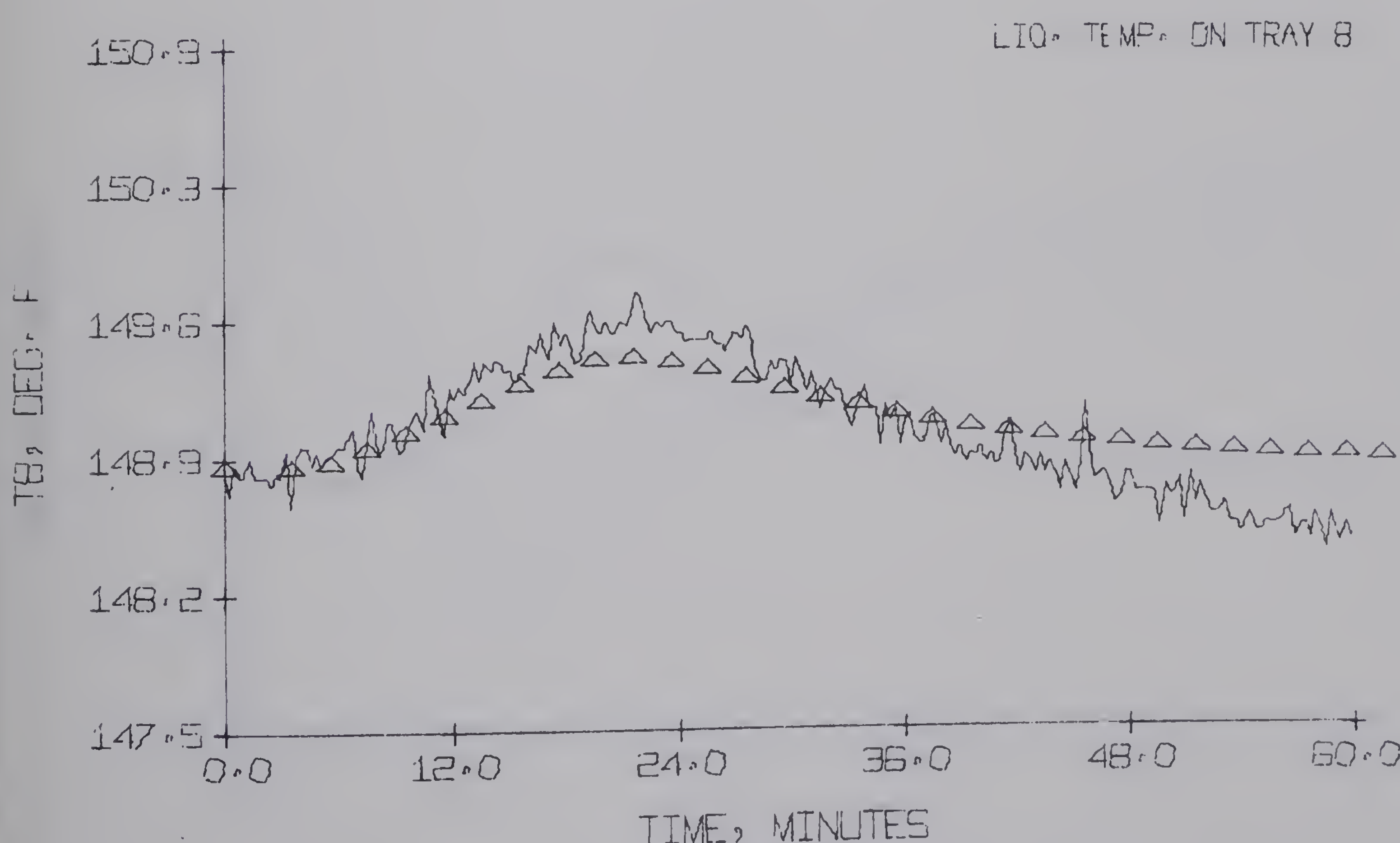

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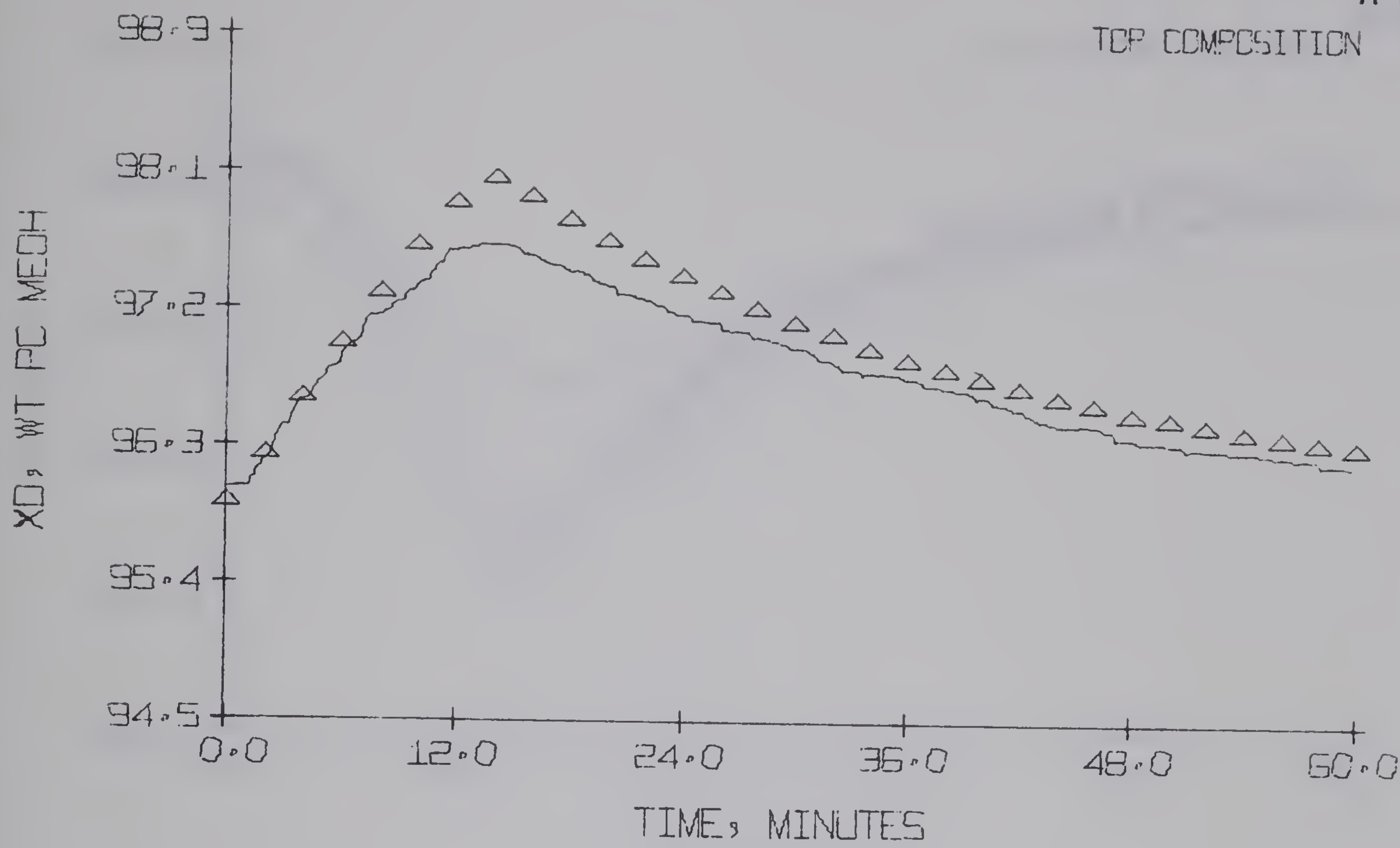

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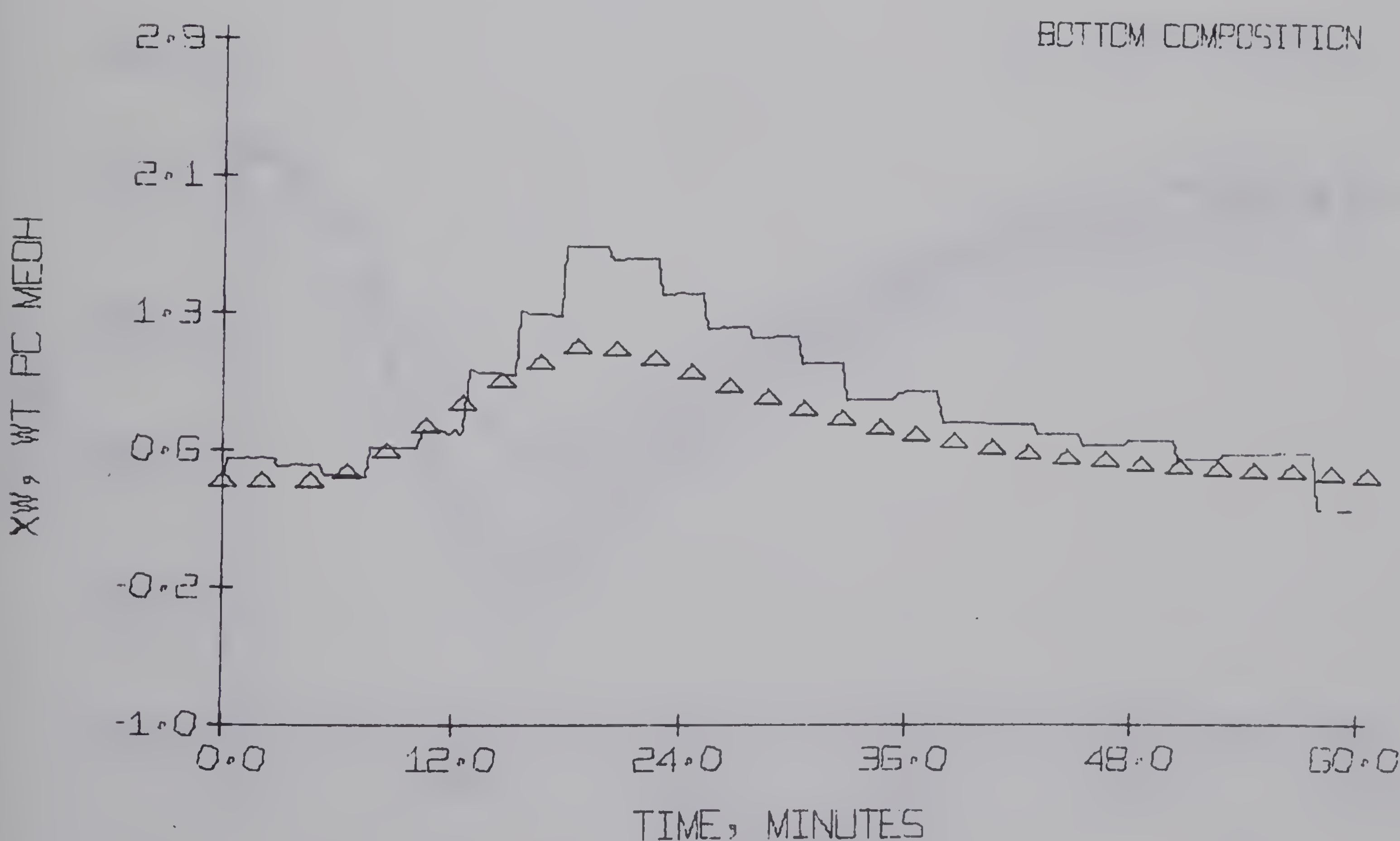

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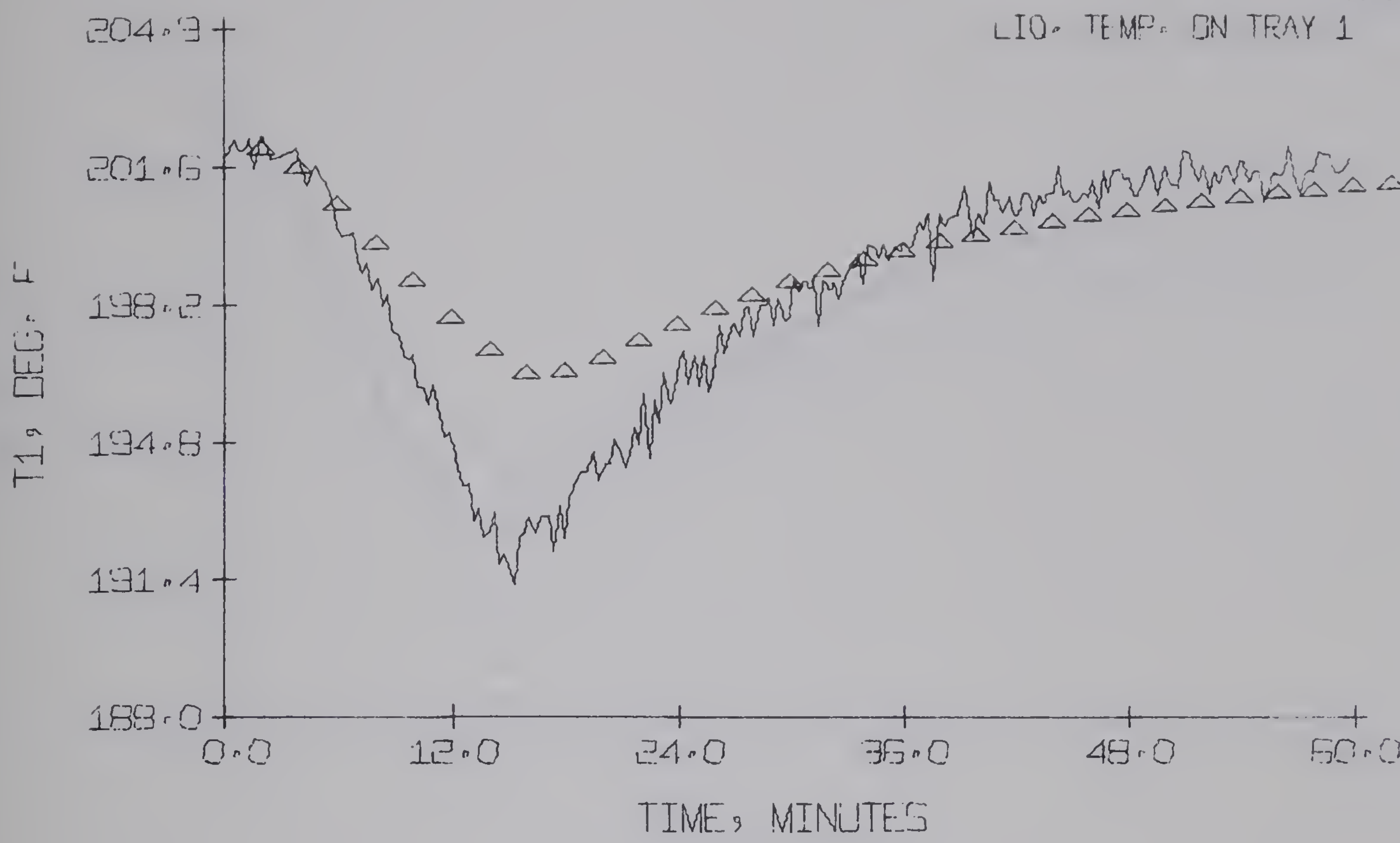

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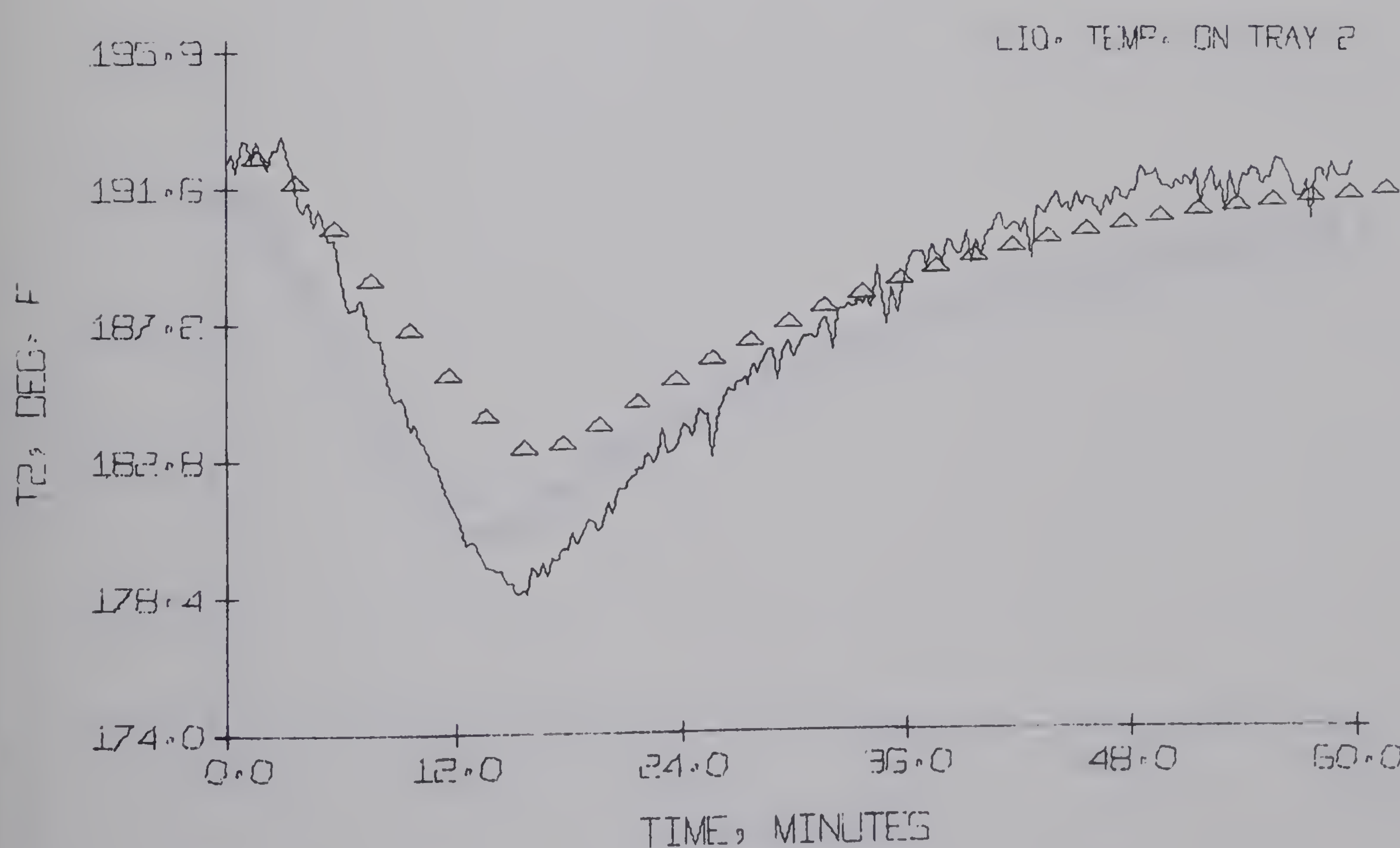

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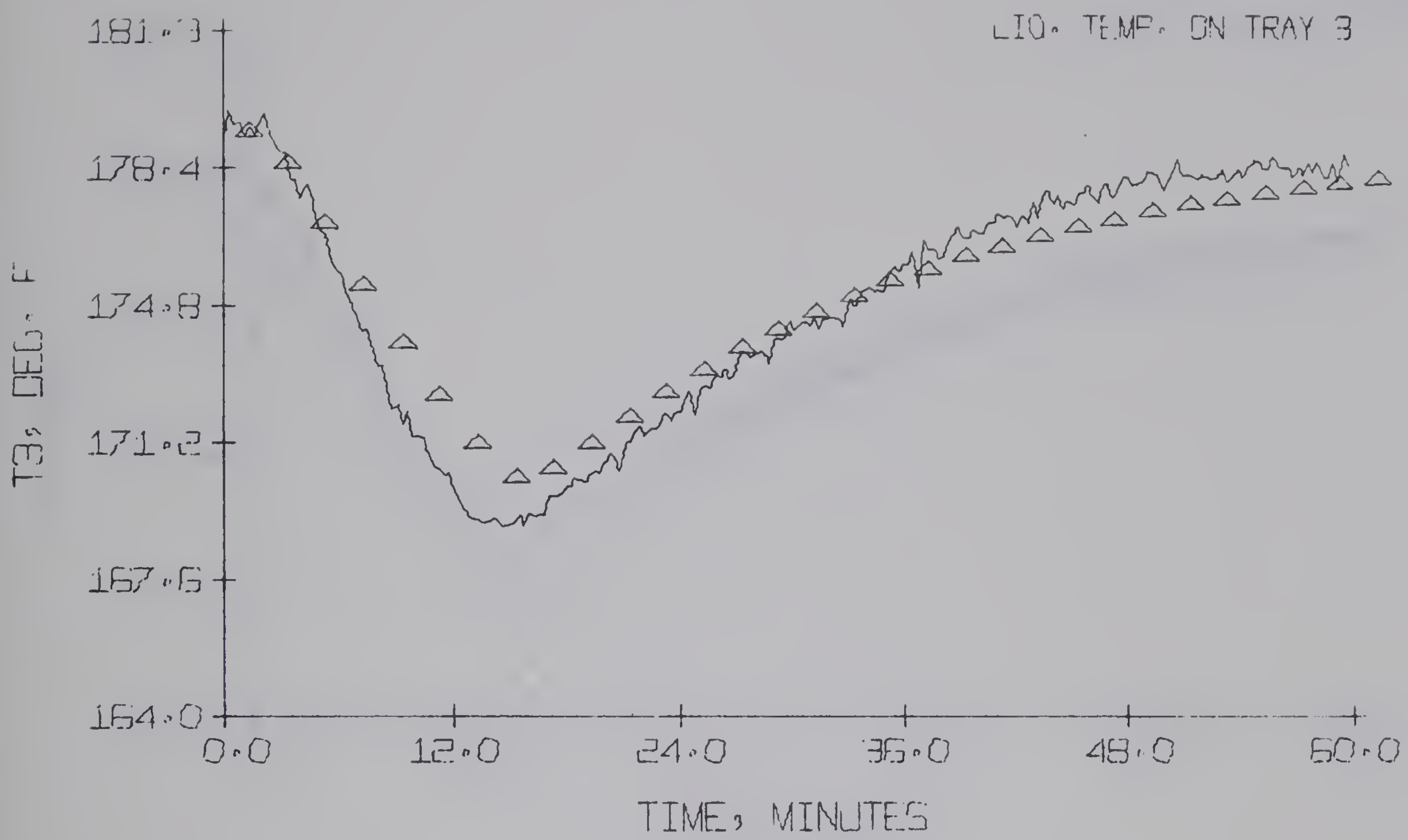

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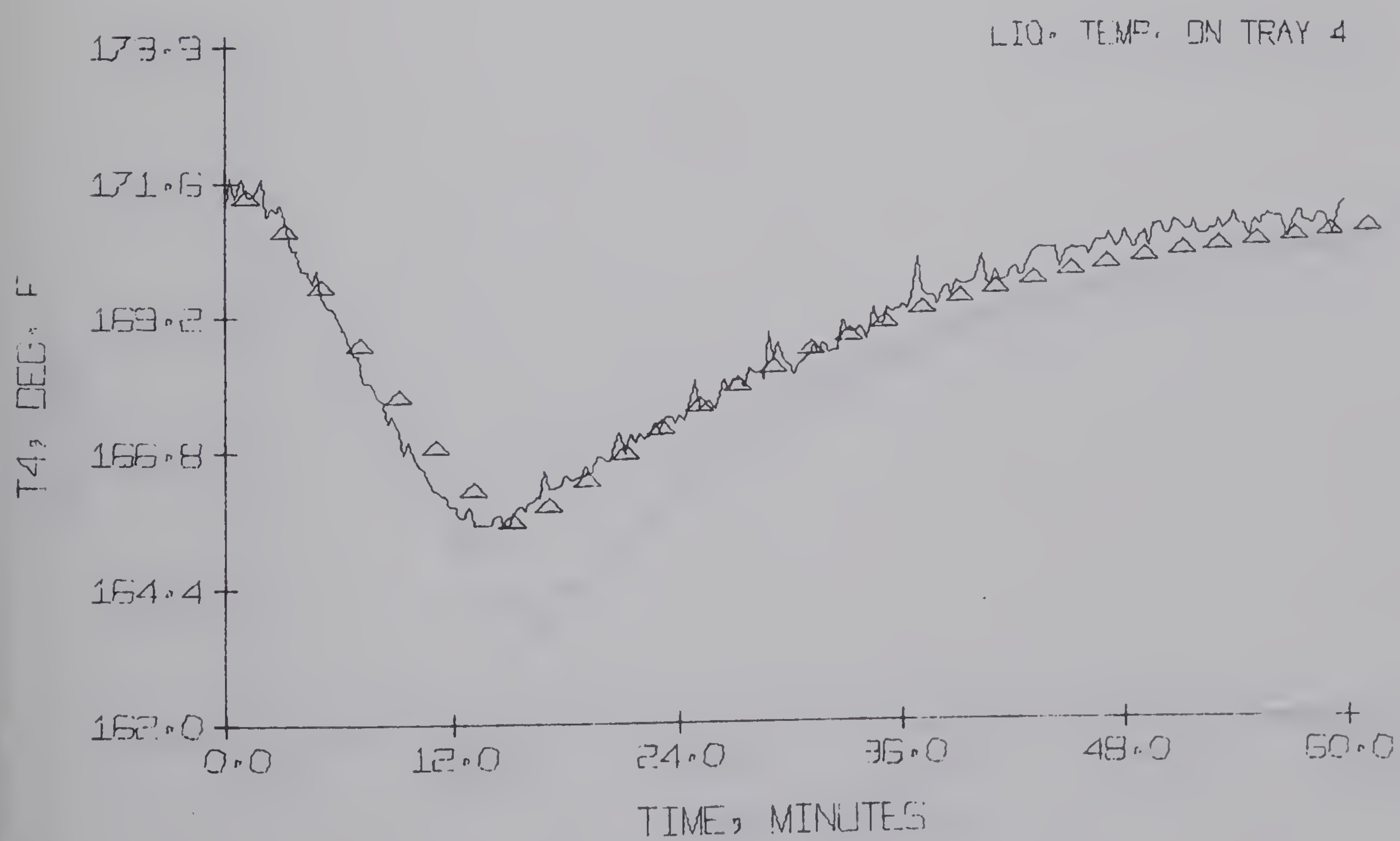

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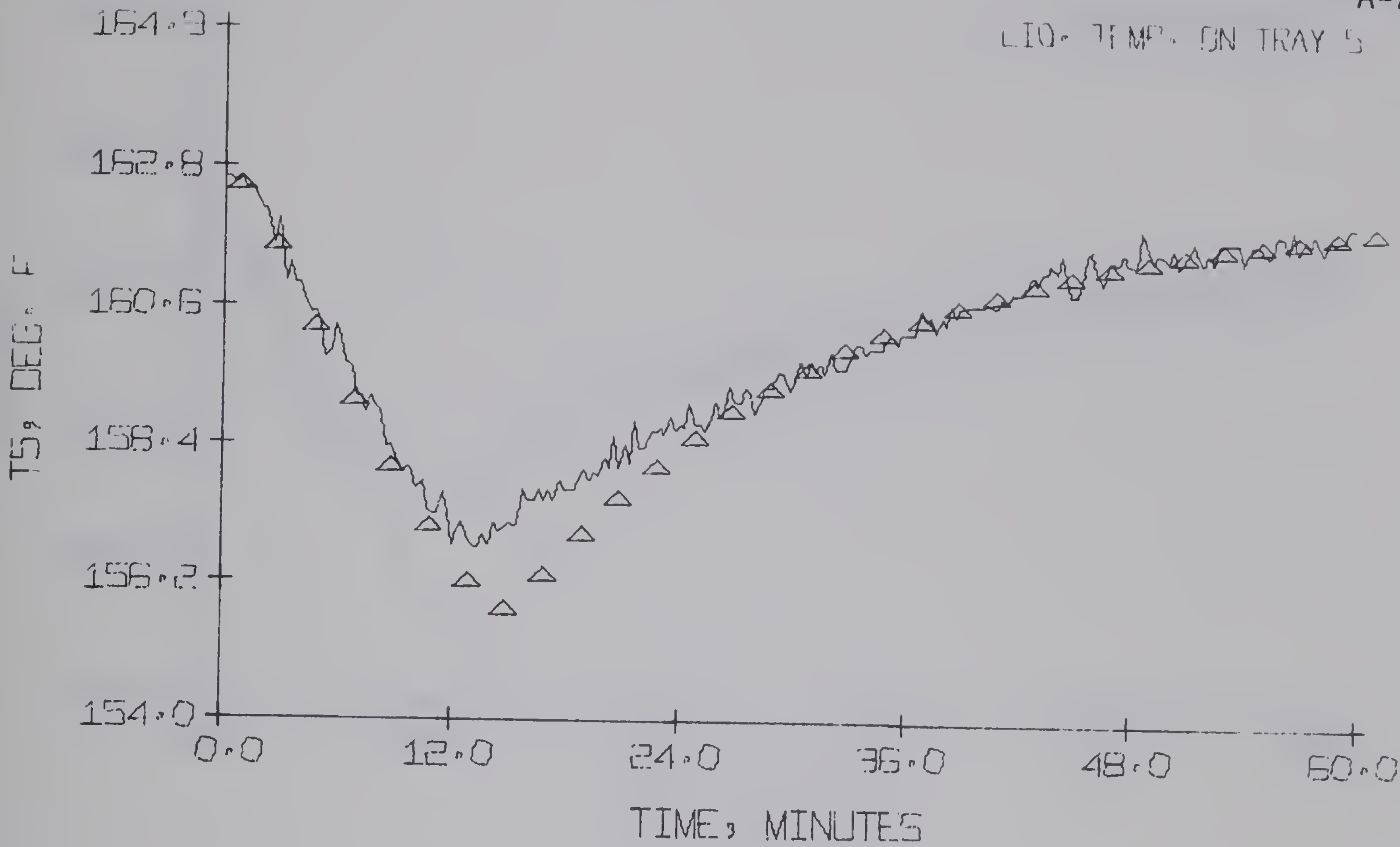

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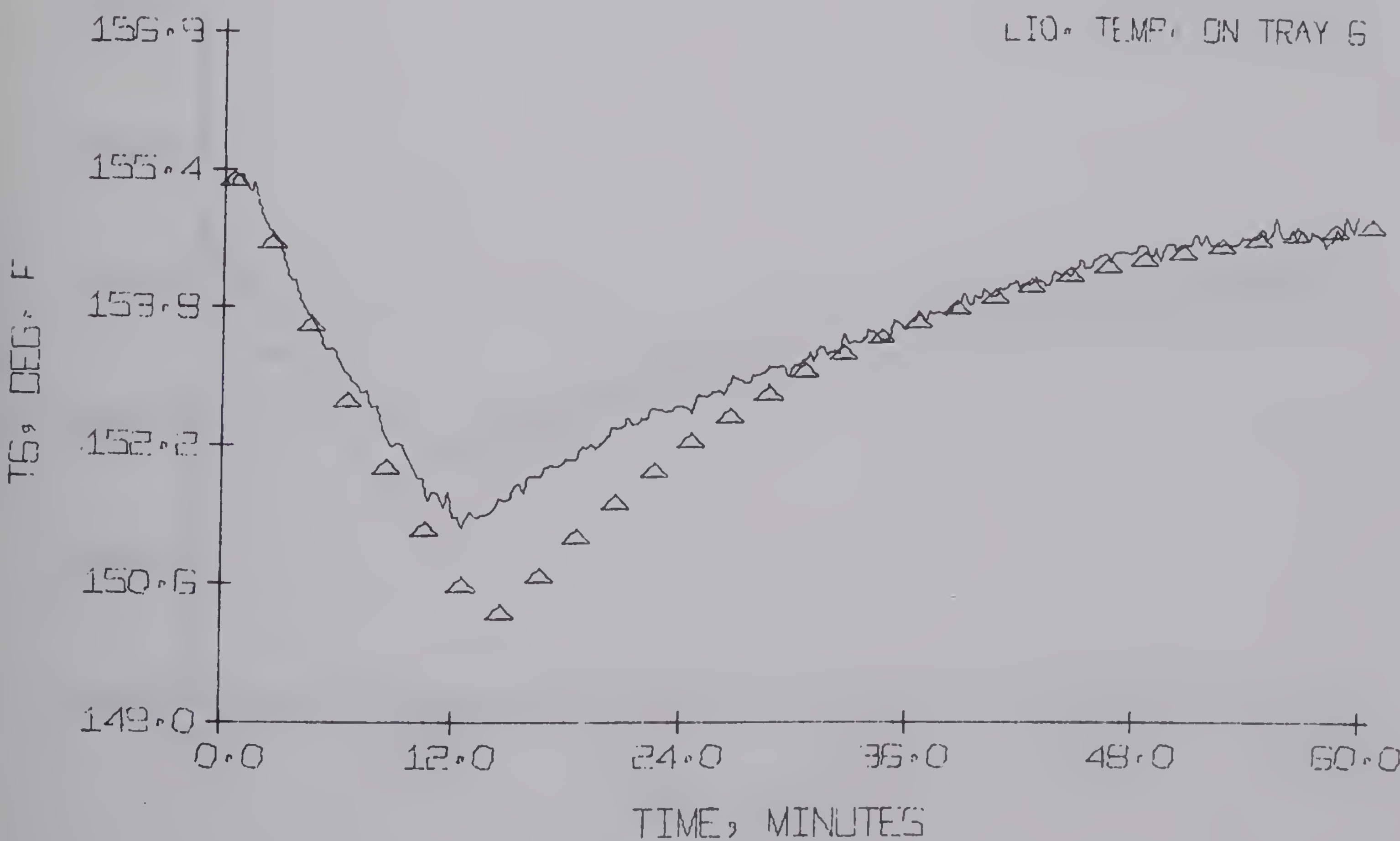

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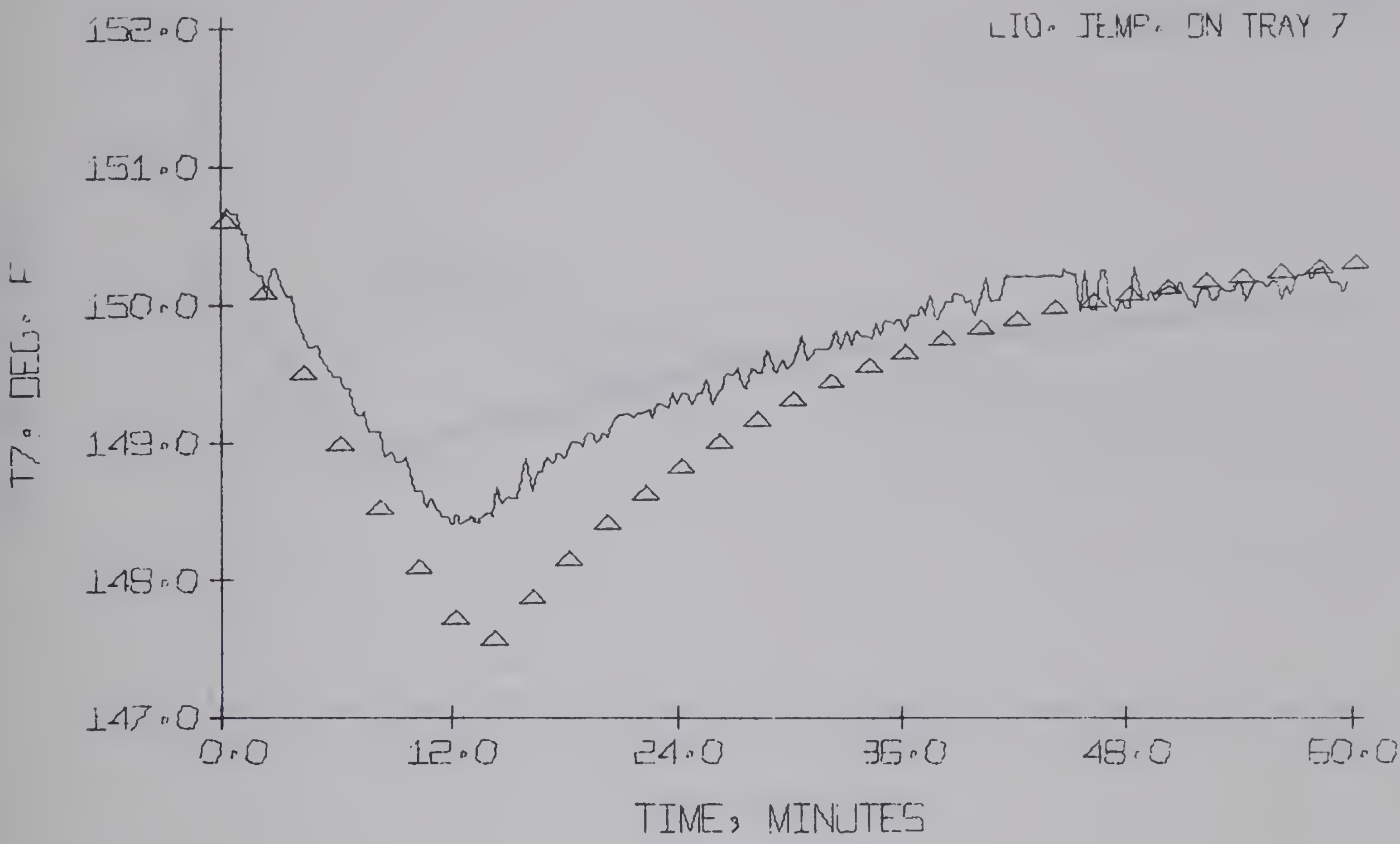

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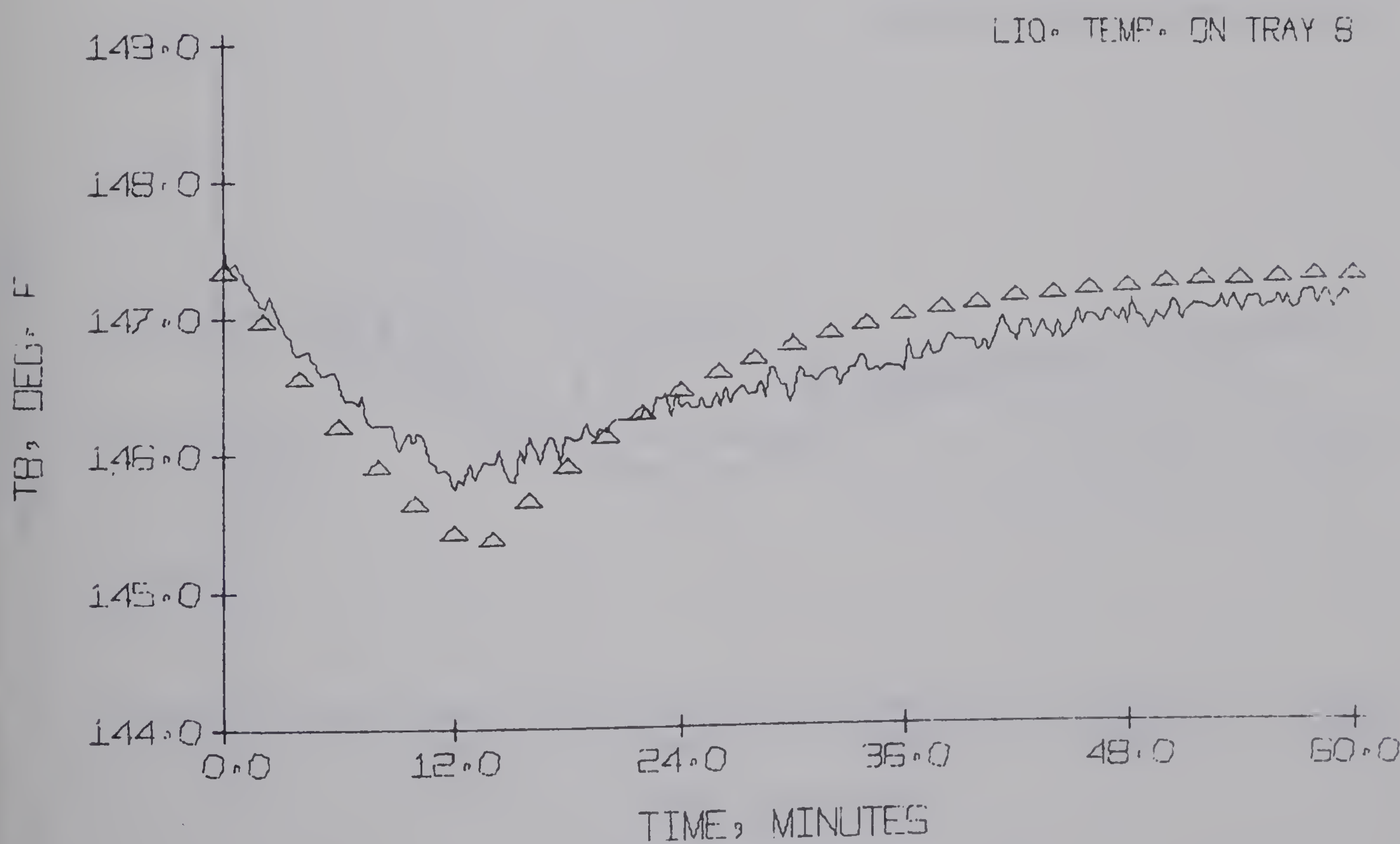

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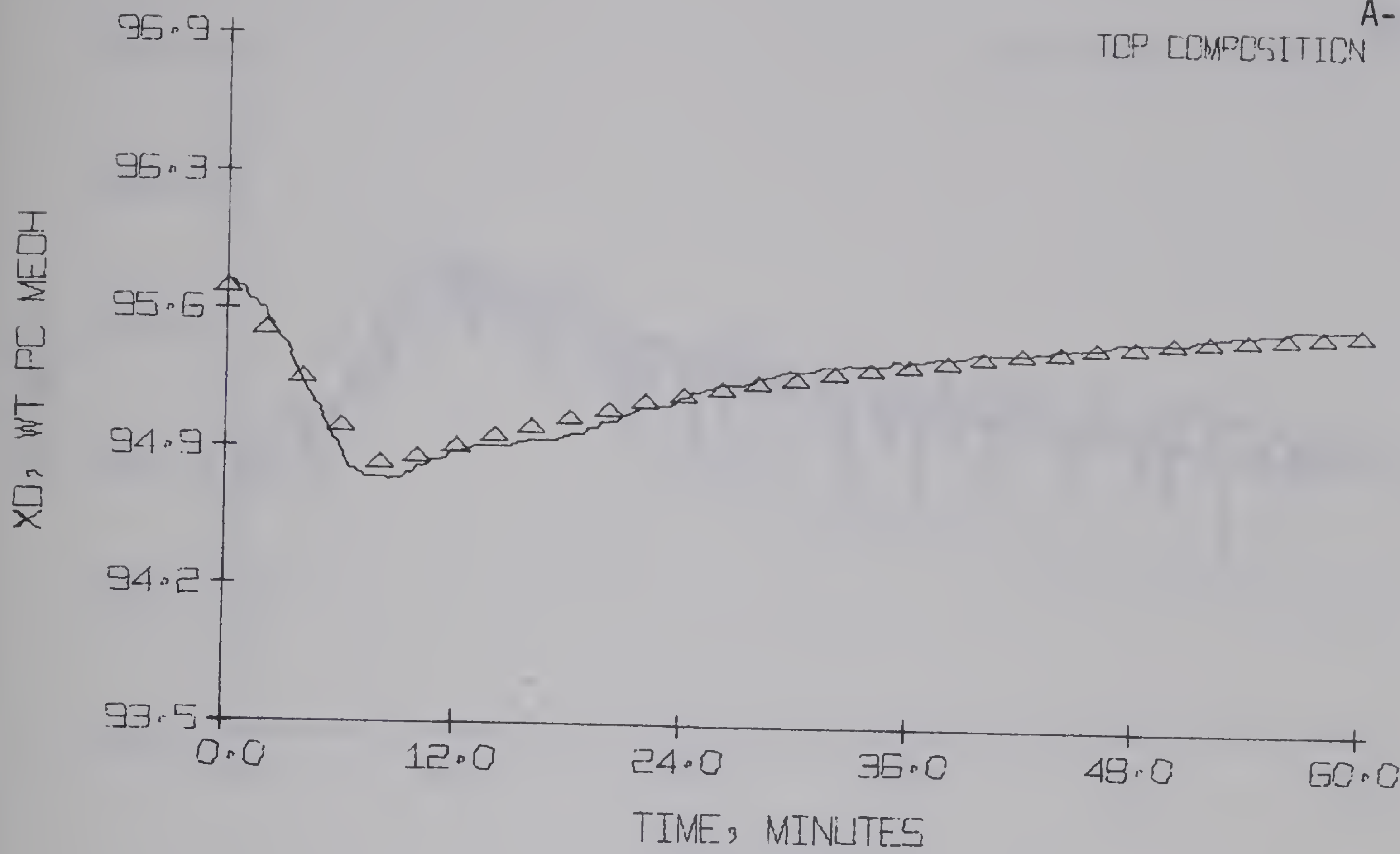

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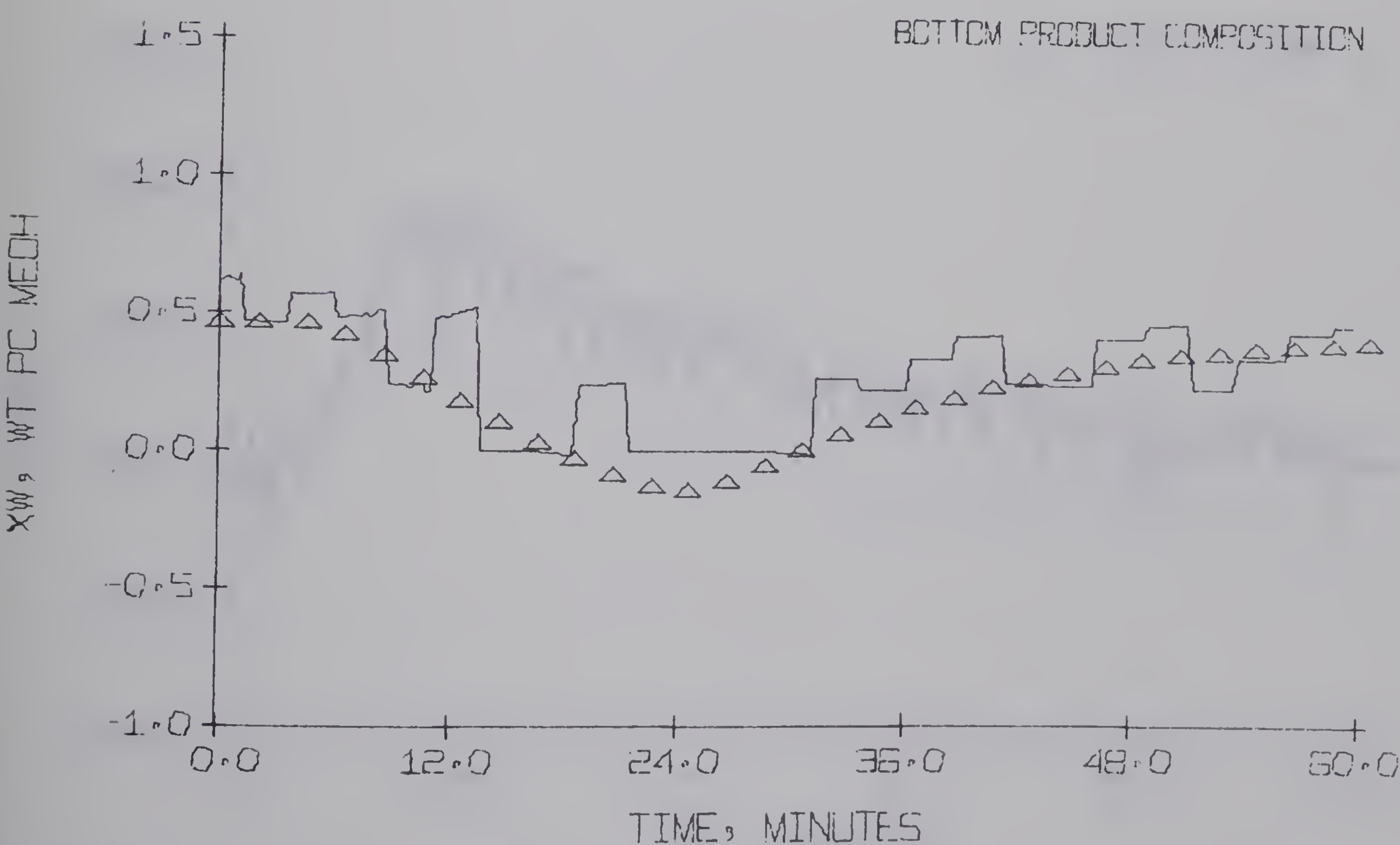

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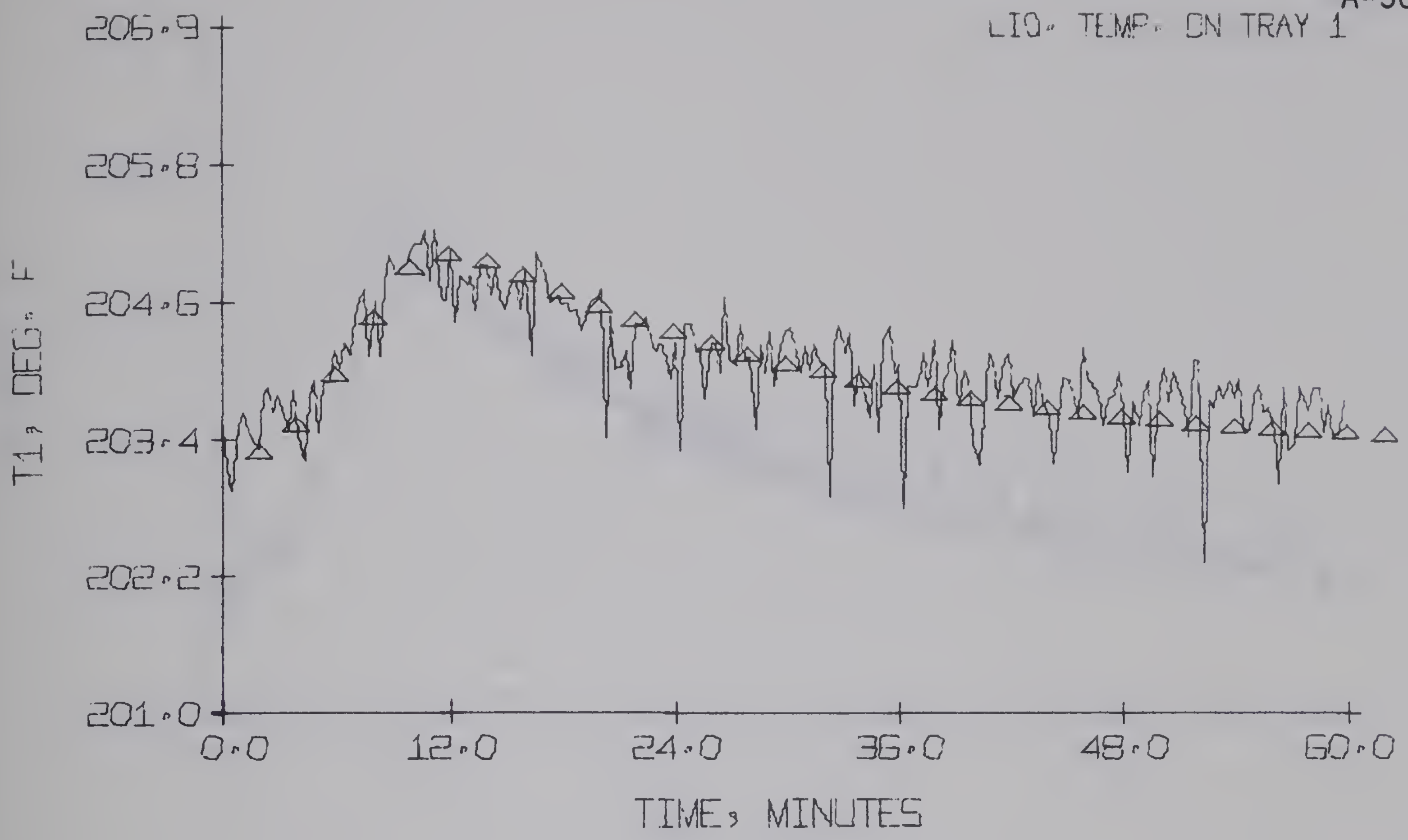

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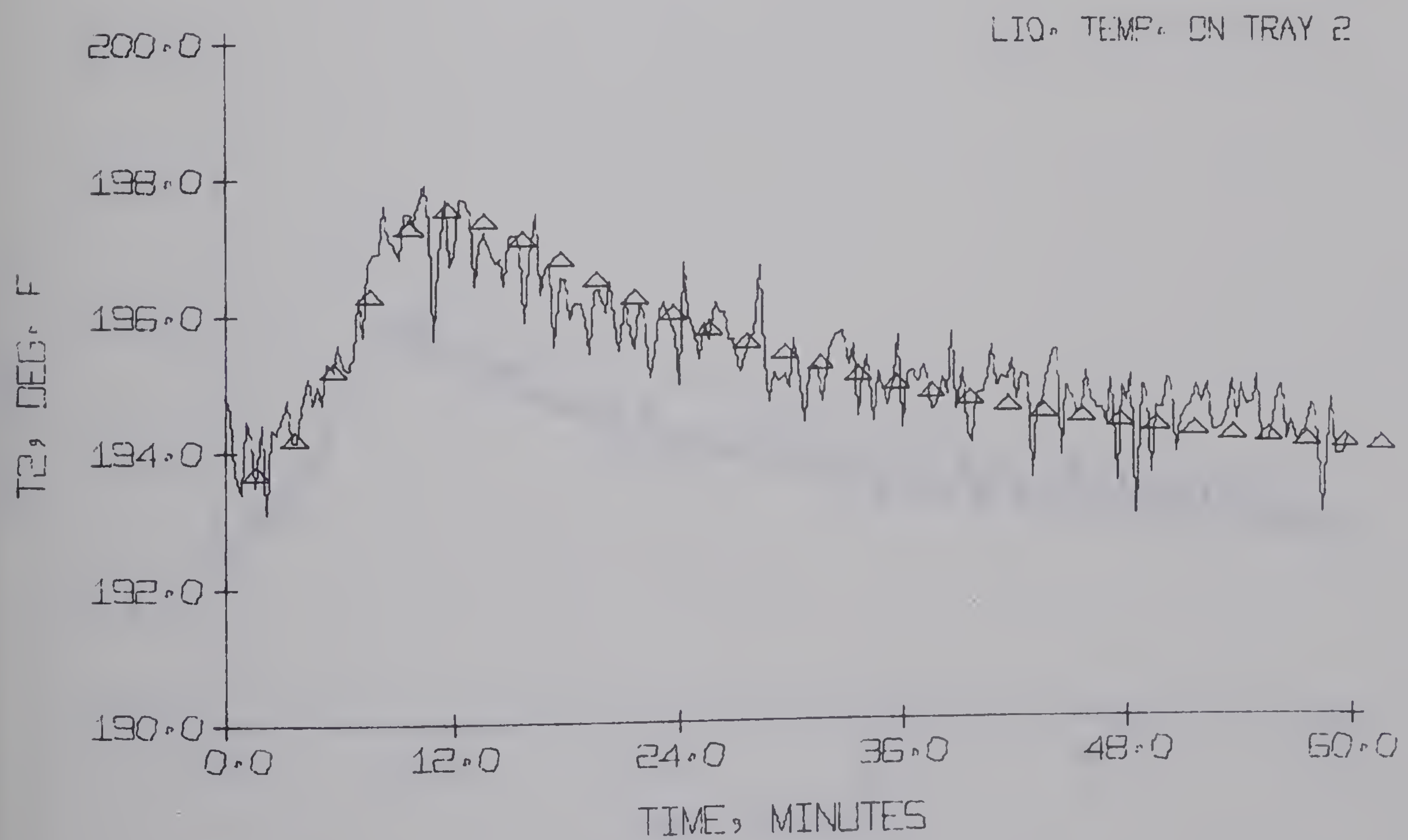

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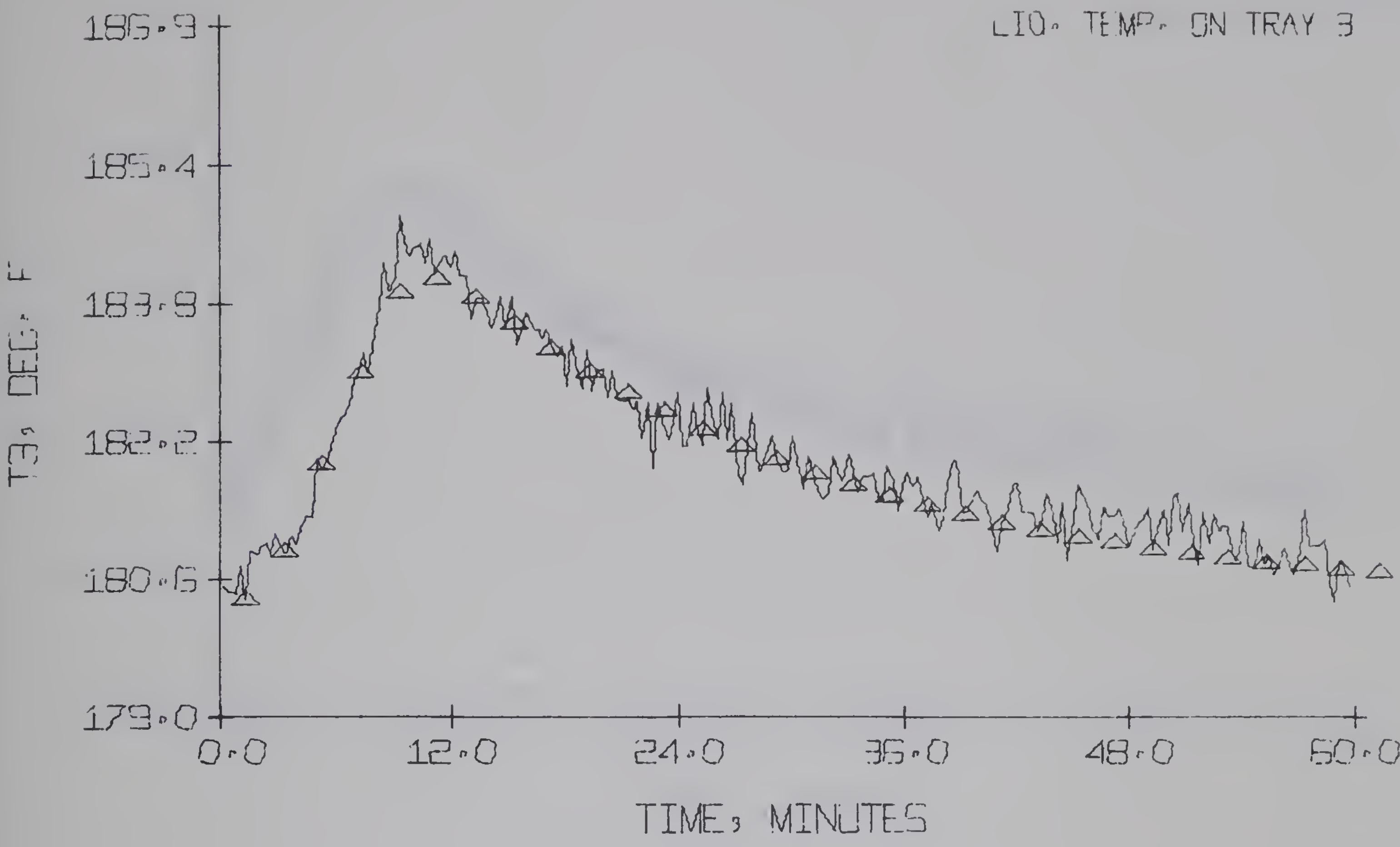

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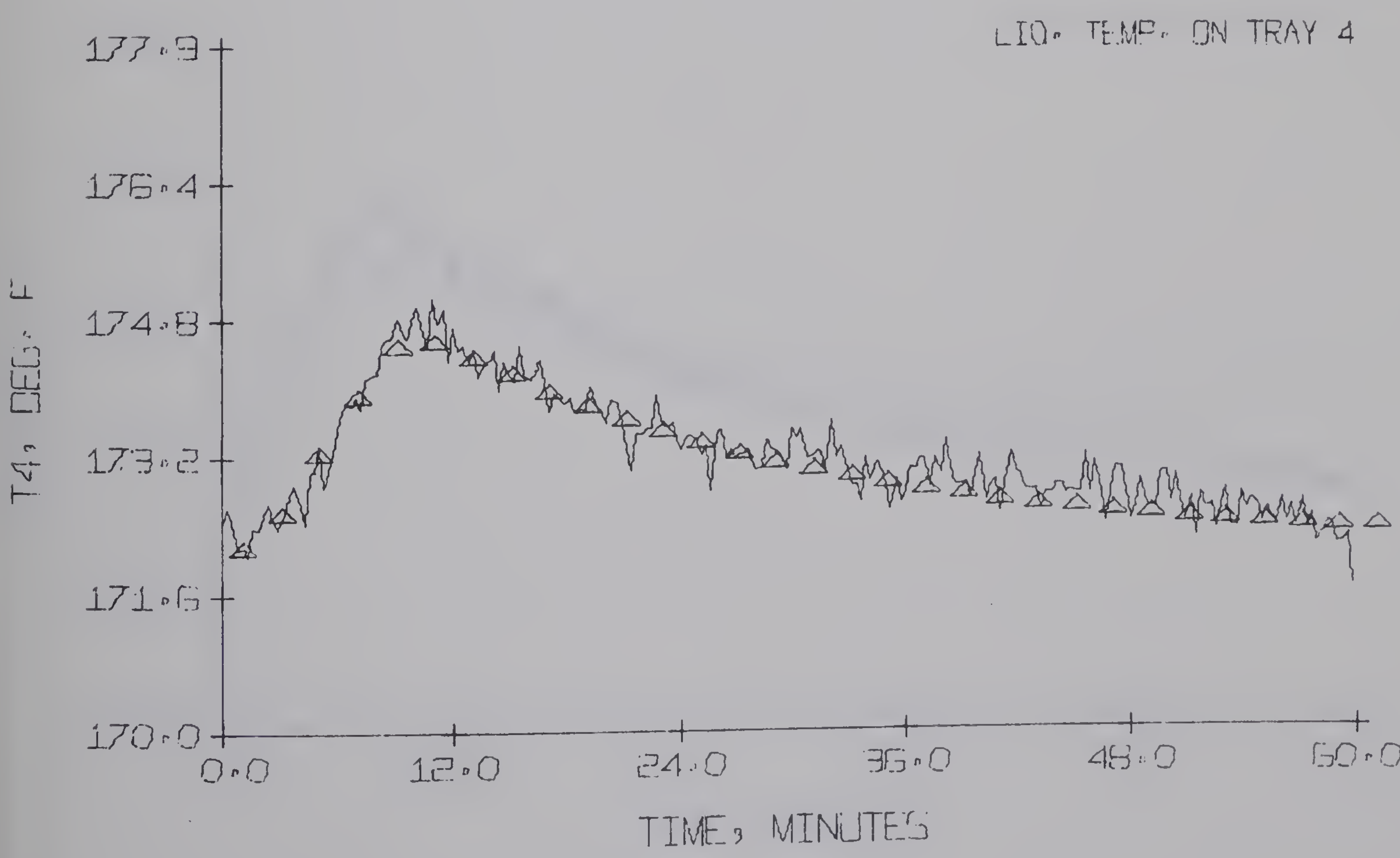

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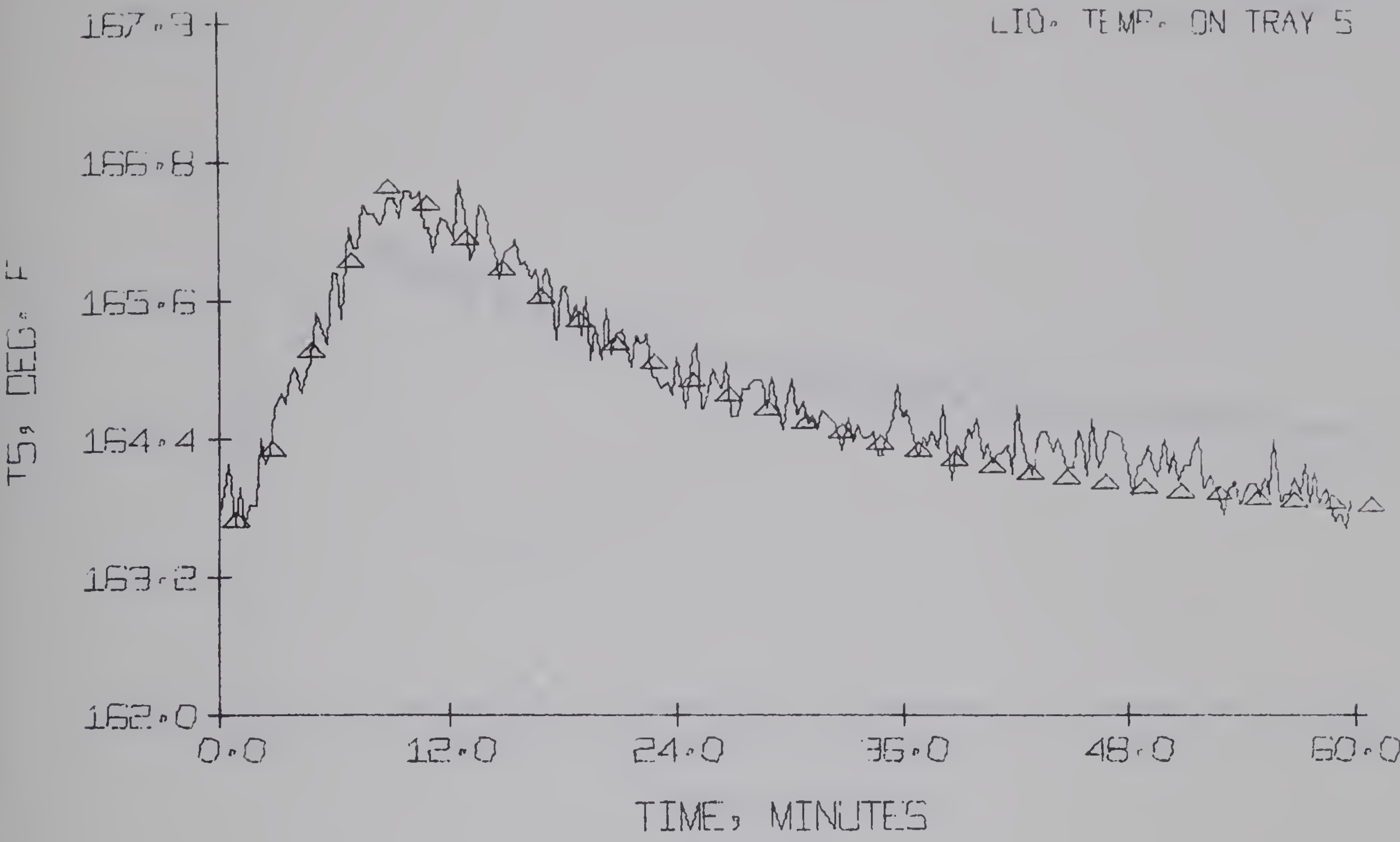

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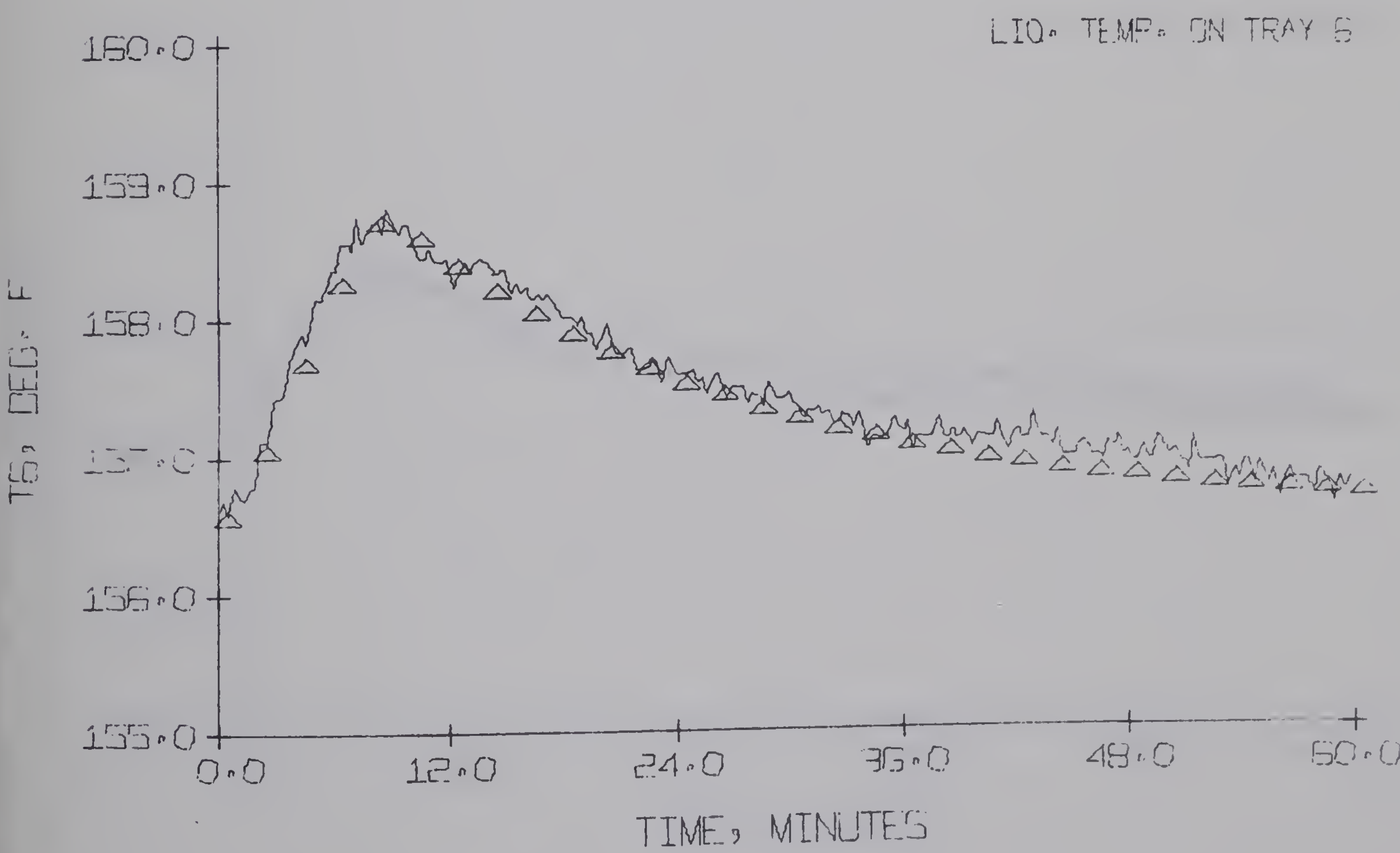

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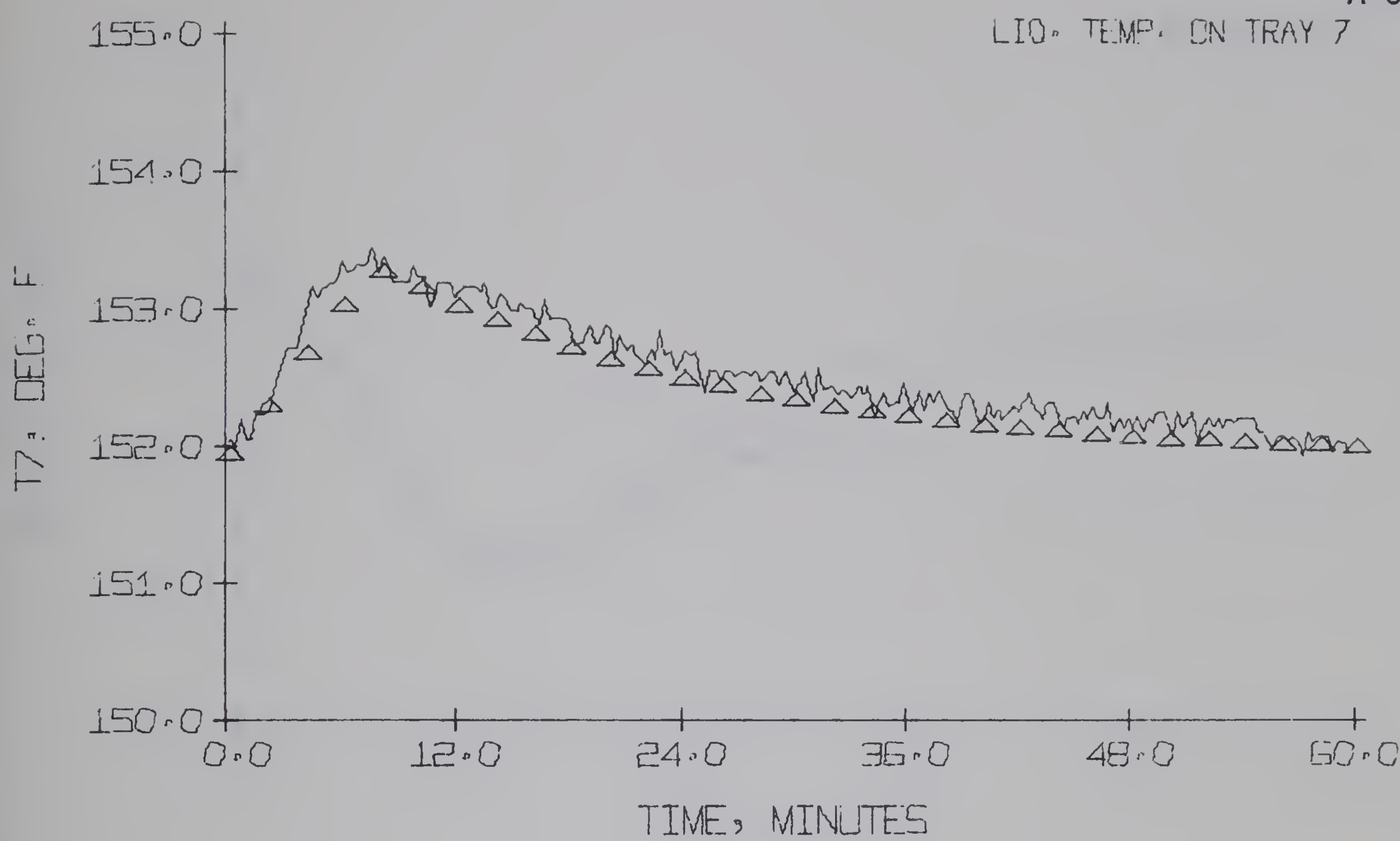

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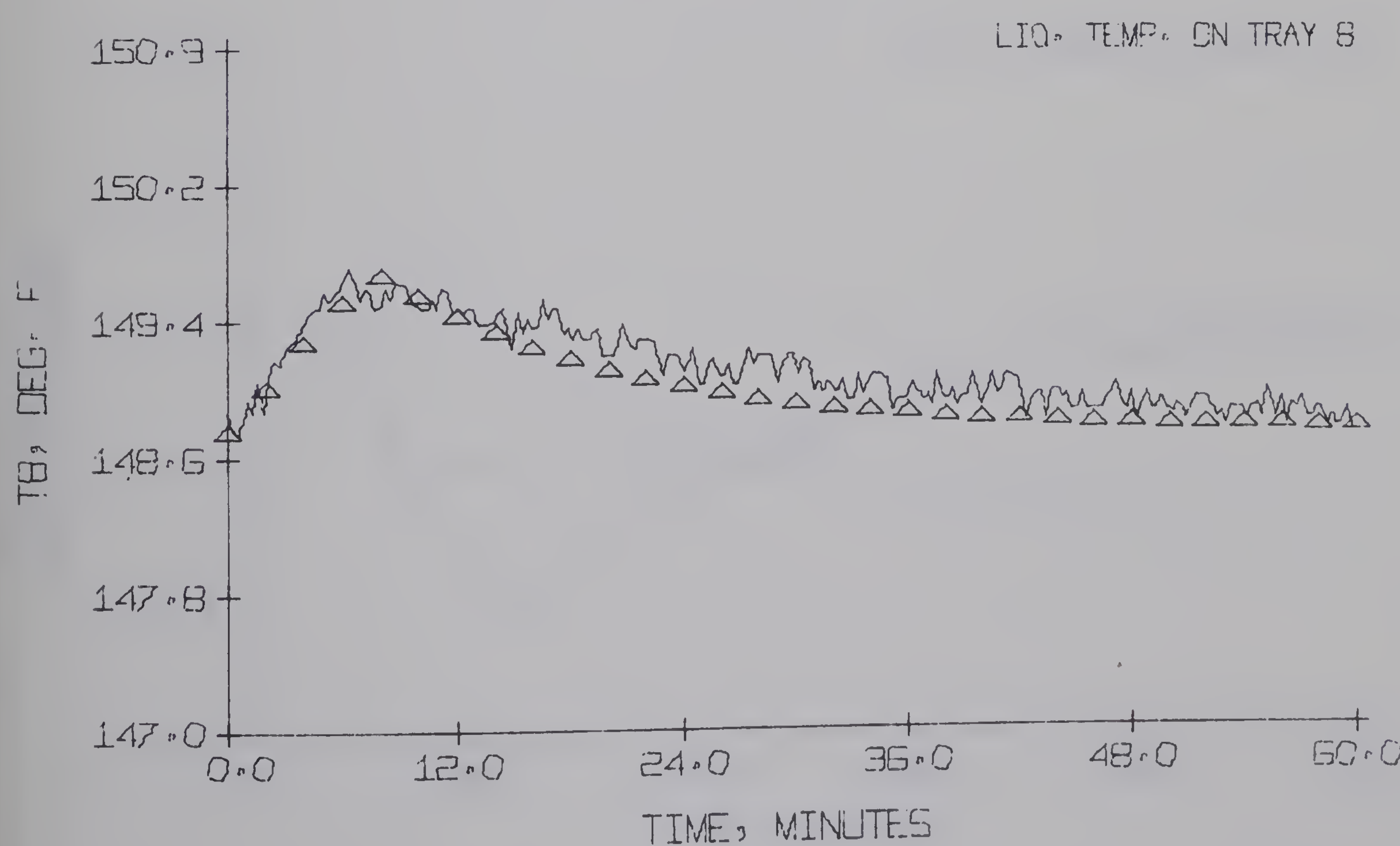

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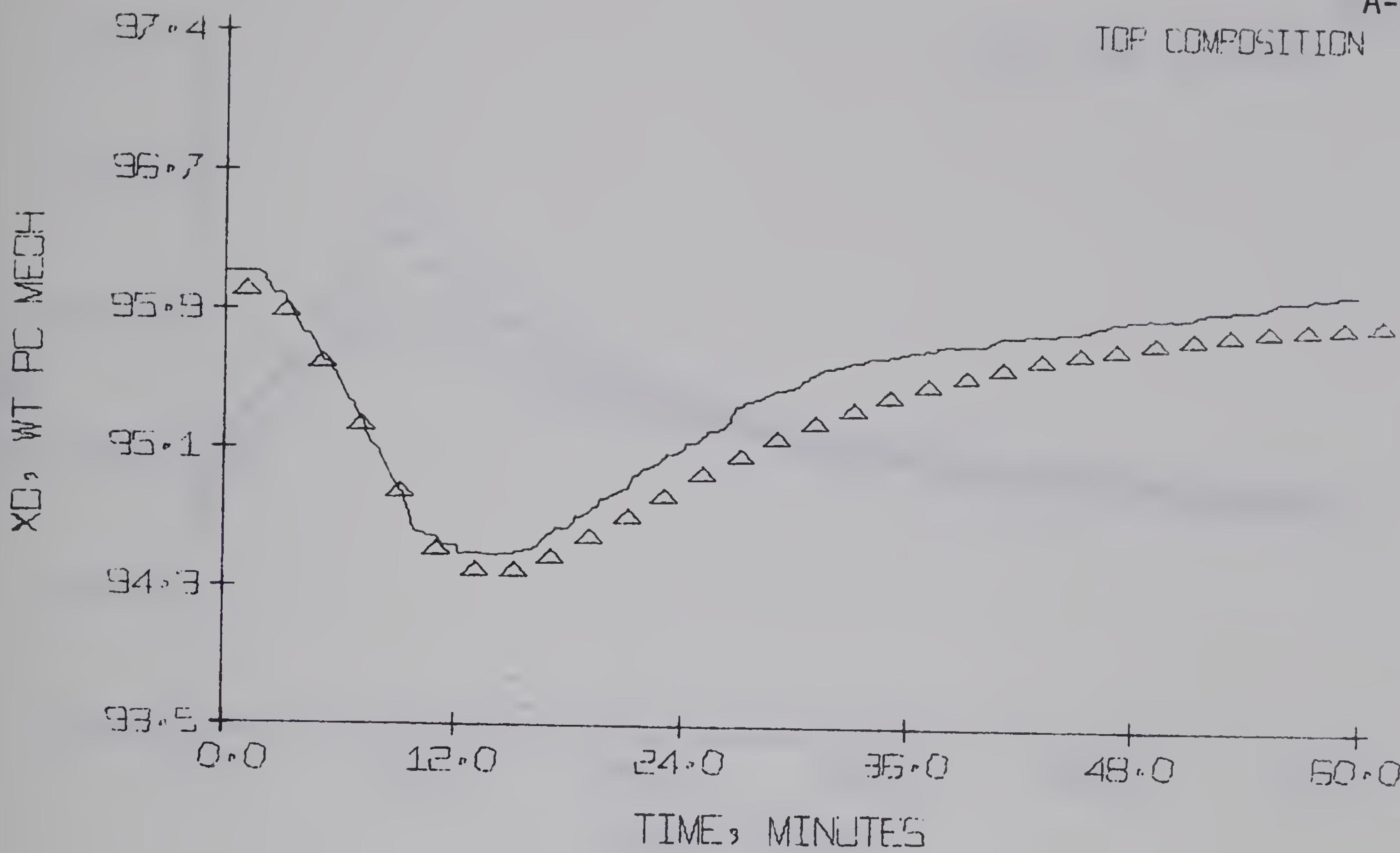

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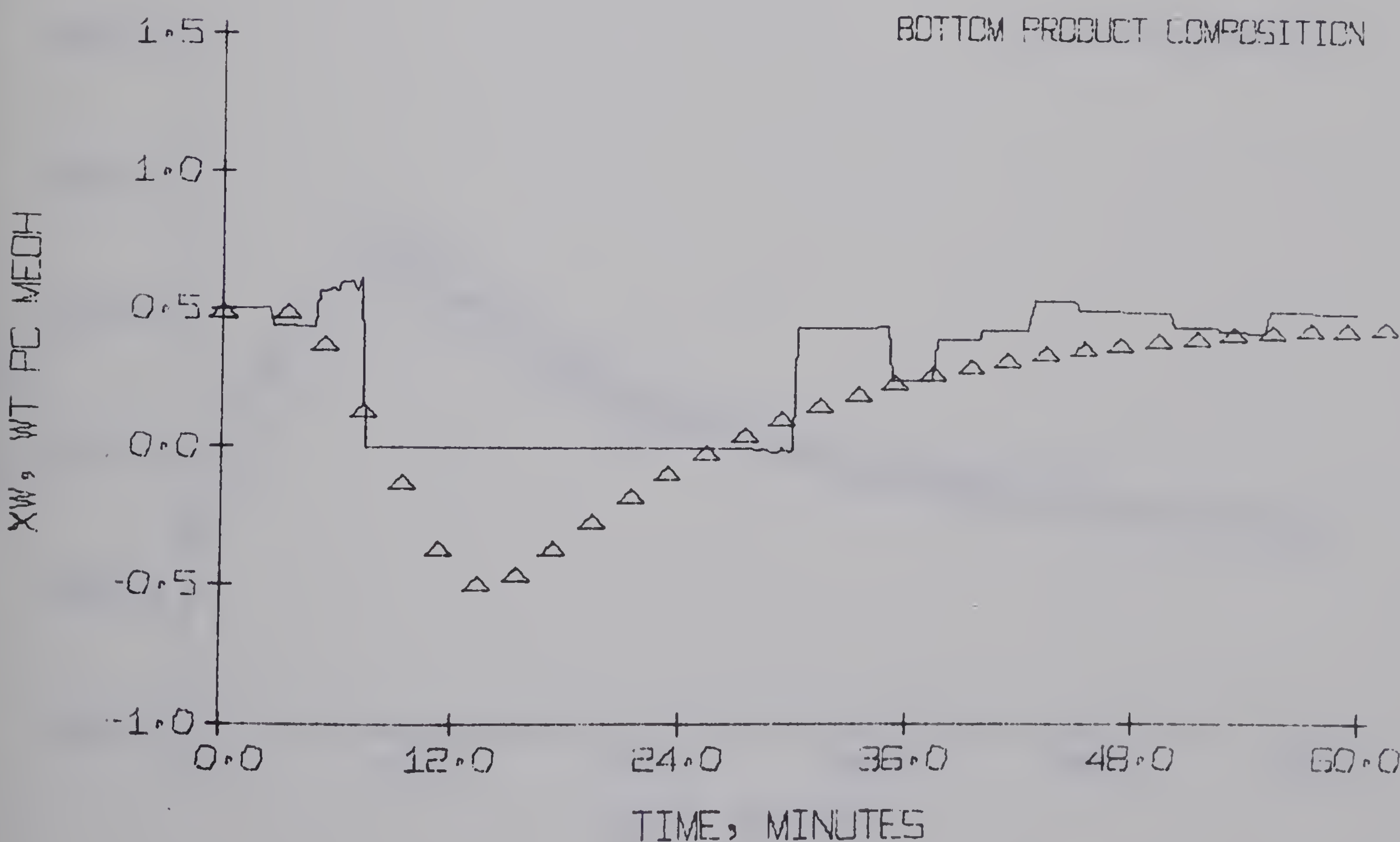

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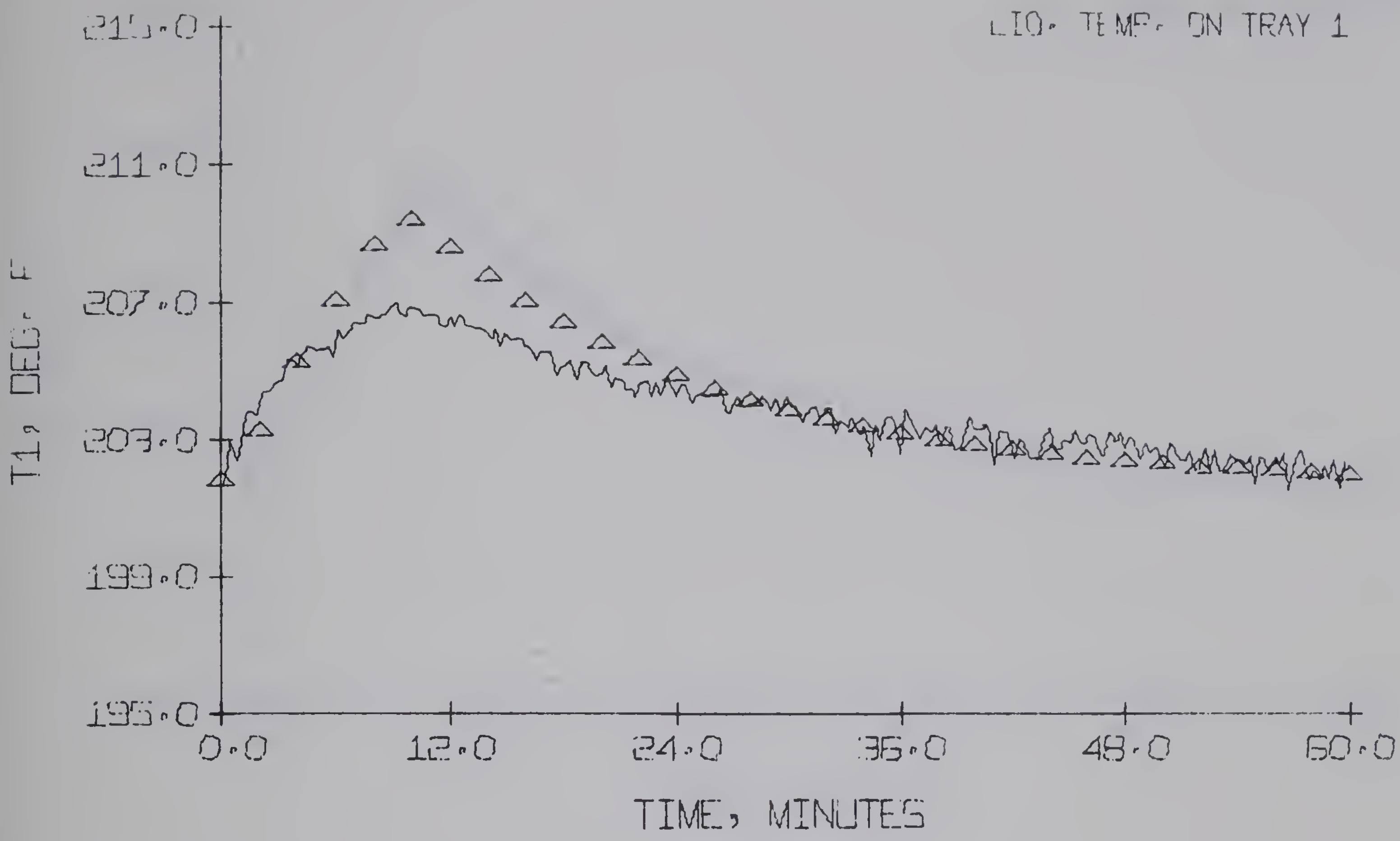

Figure A.2-43

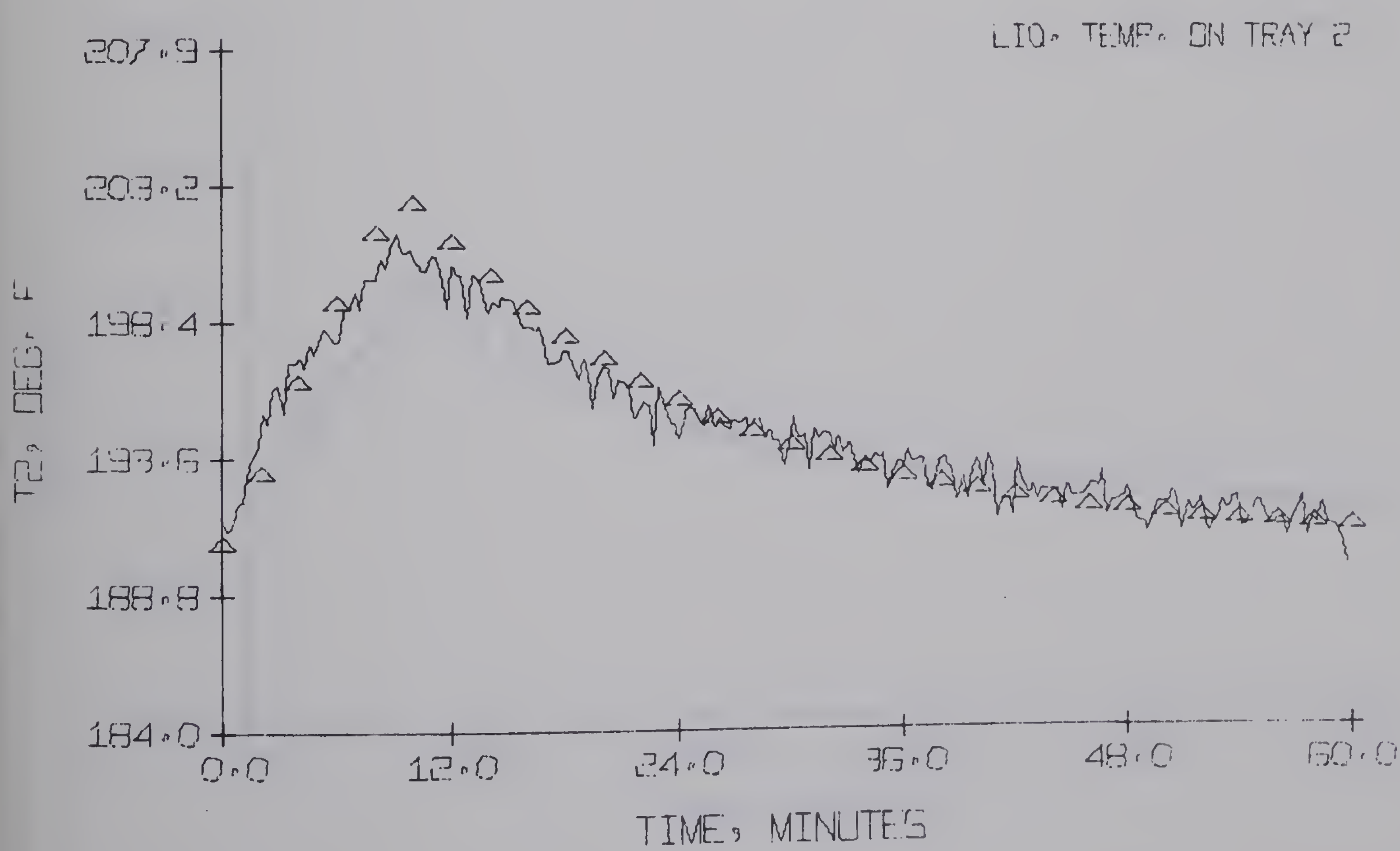

Figure A.2-44

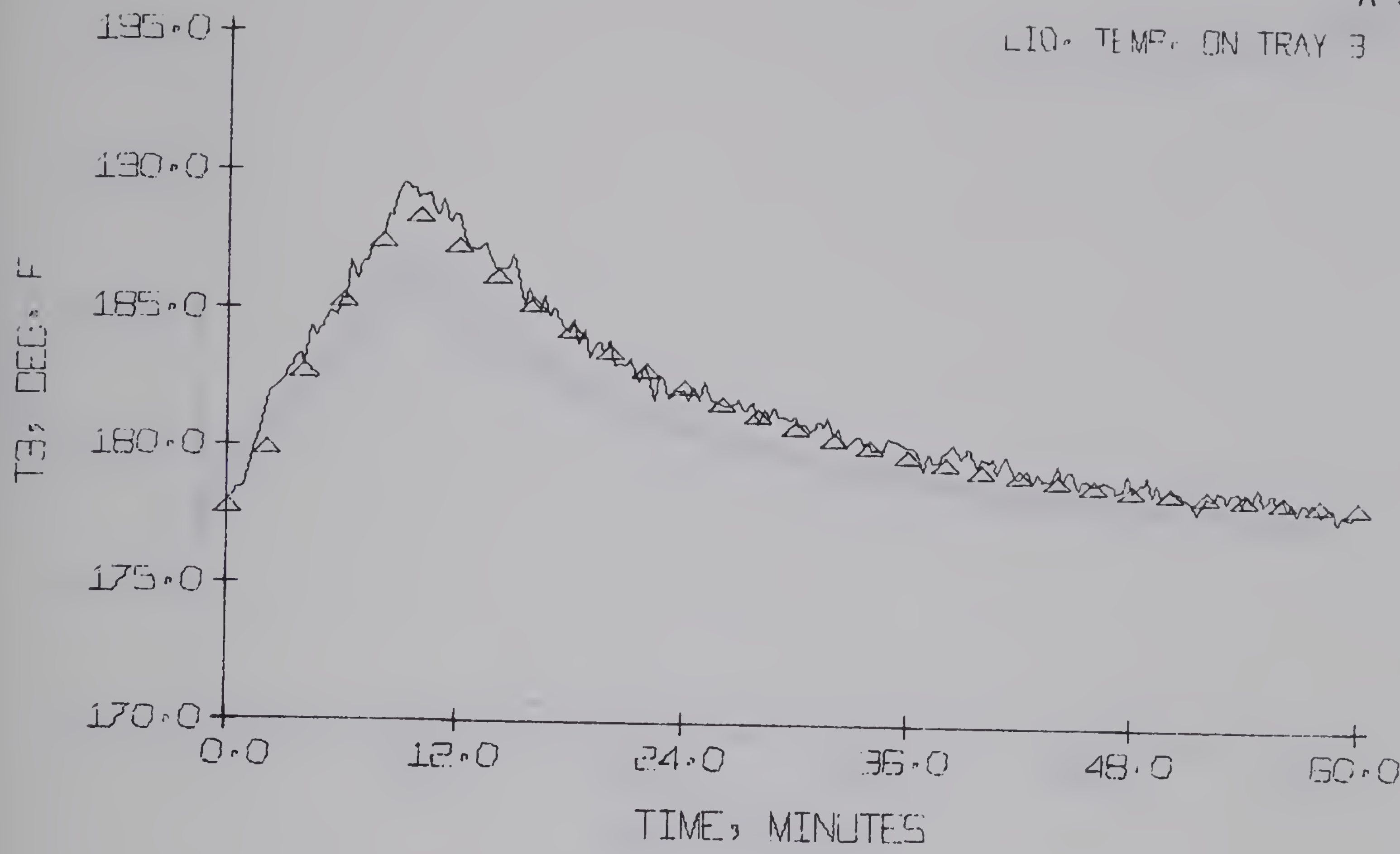

Figure A.2-45

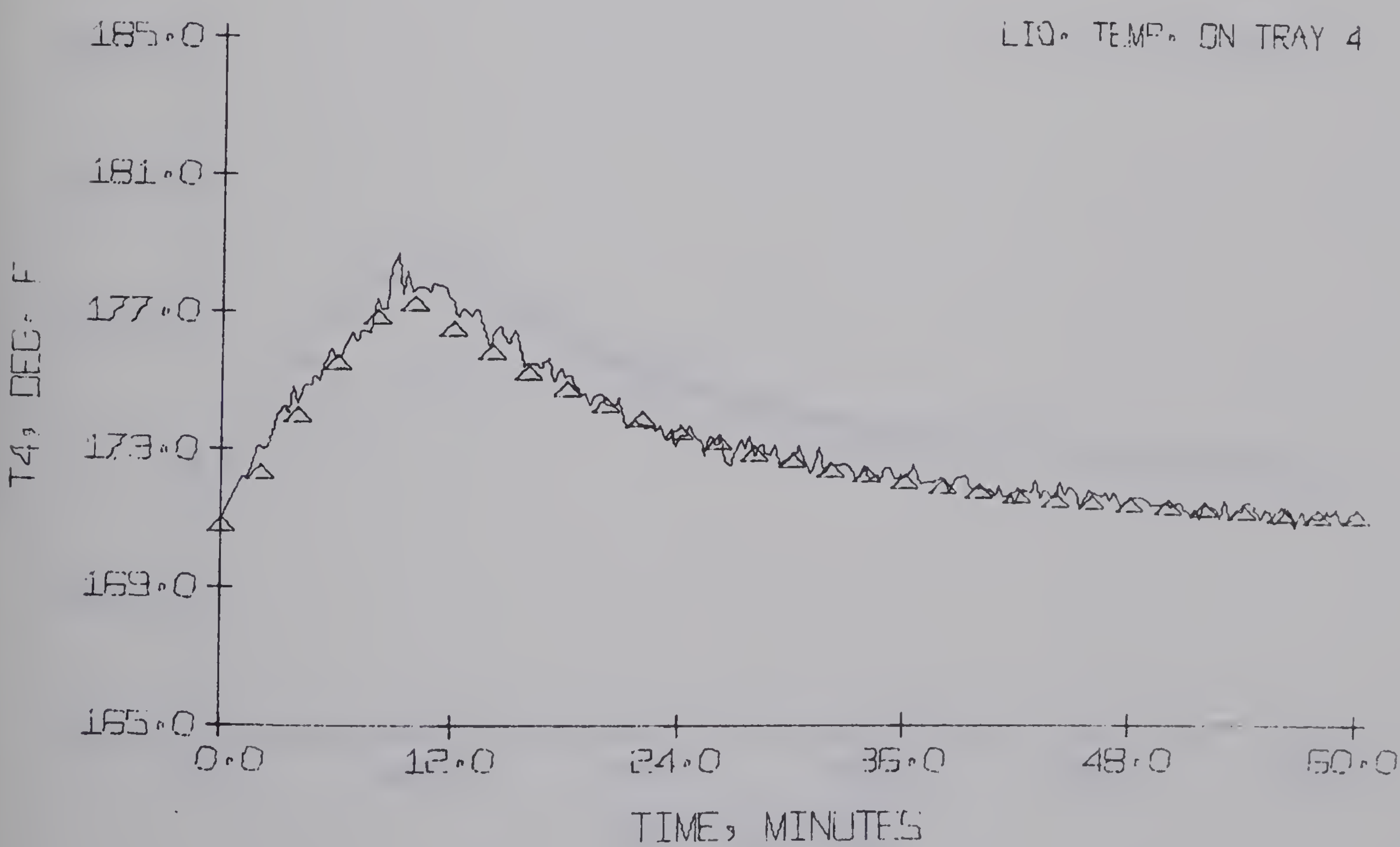

Figure A.2-46

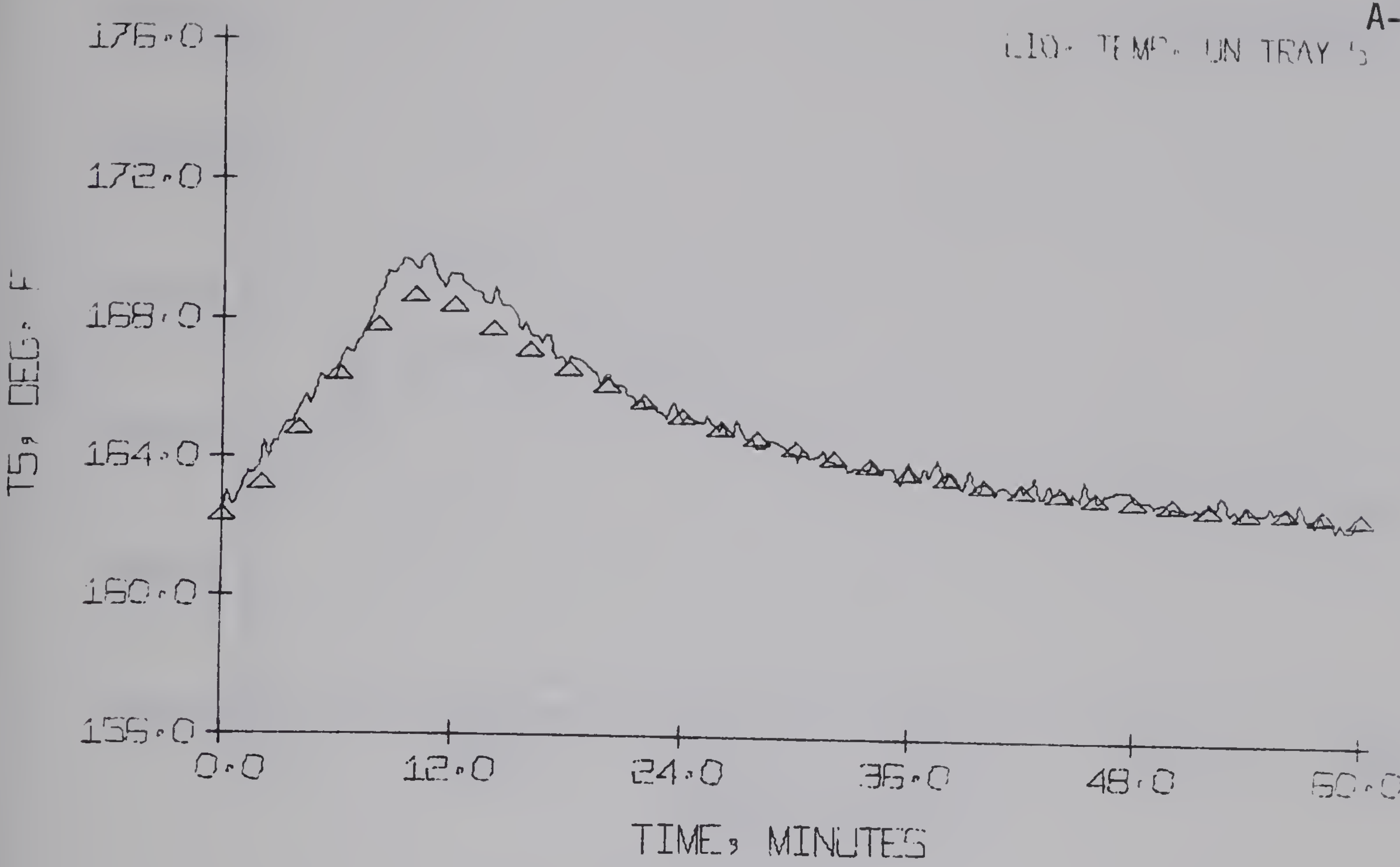

Figure A.2-47

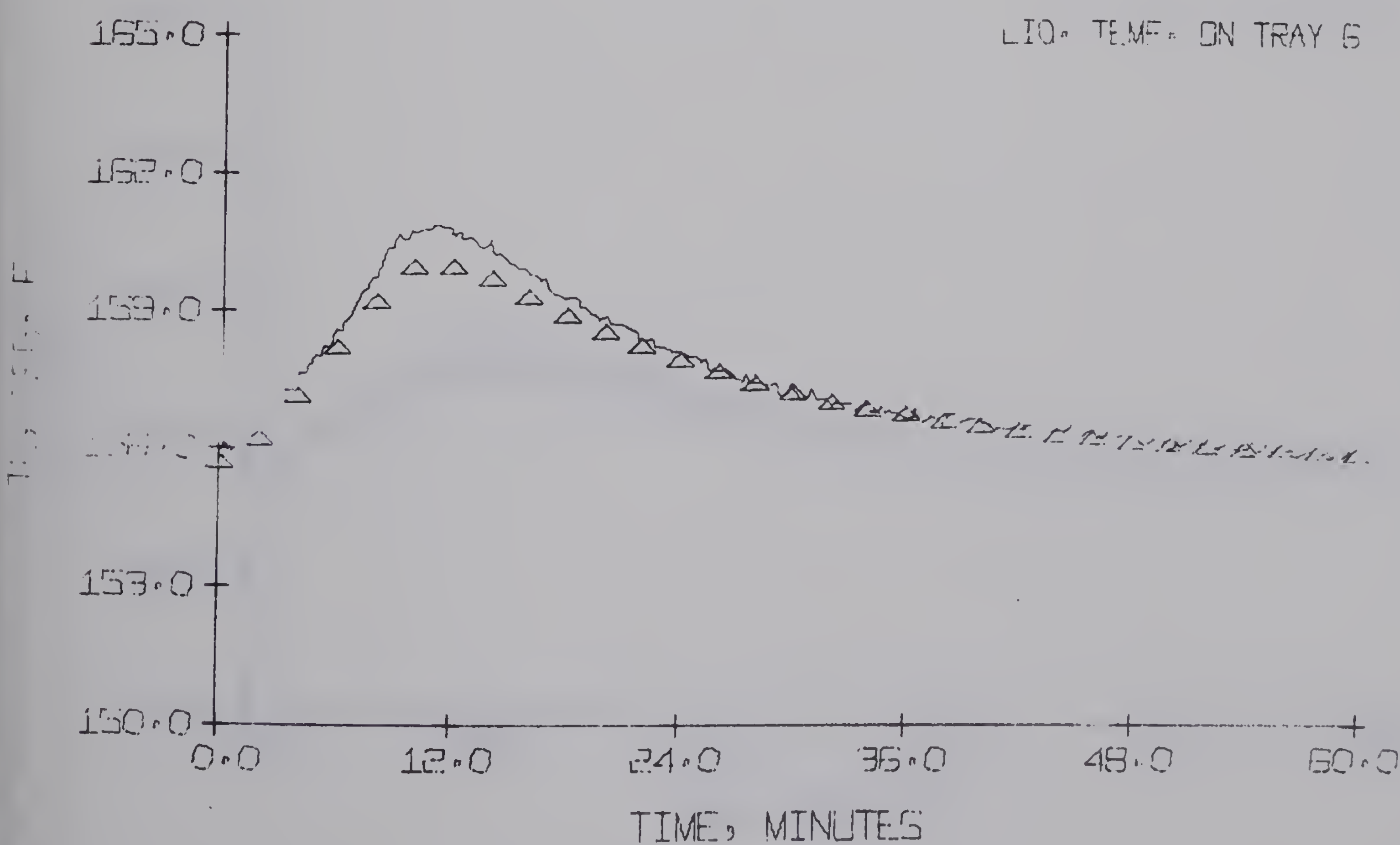

Figure A.2-48

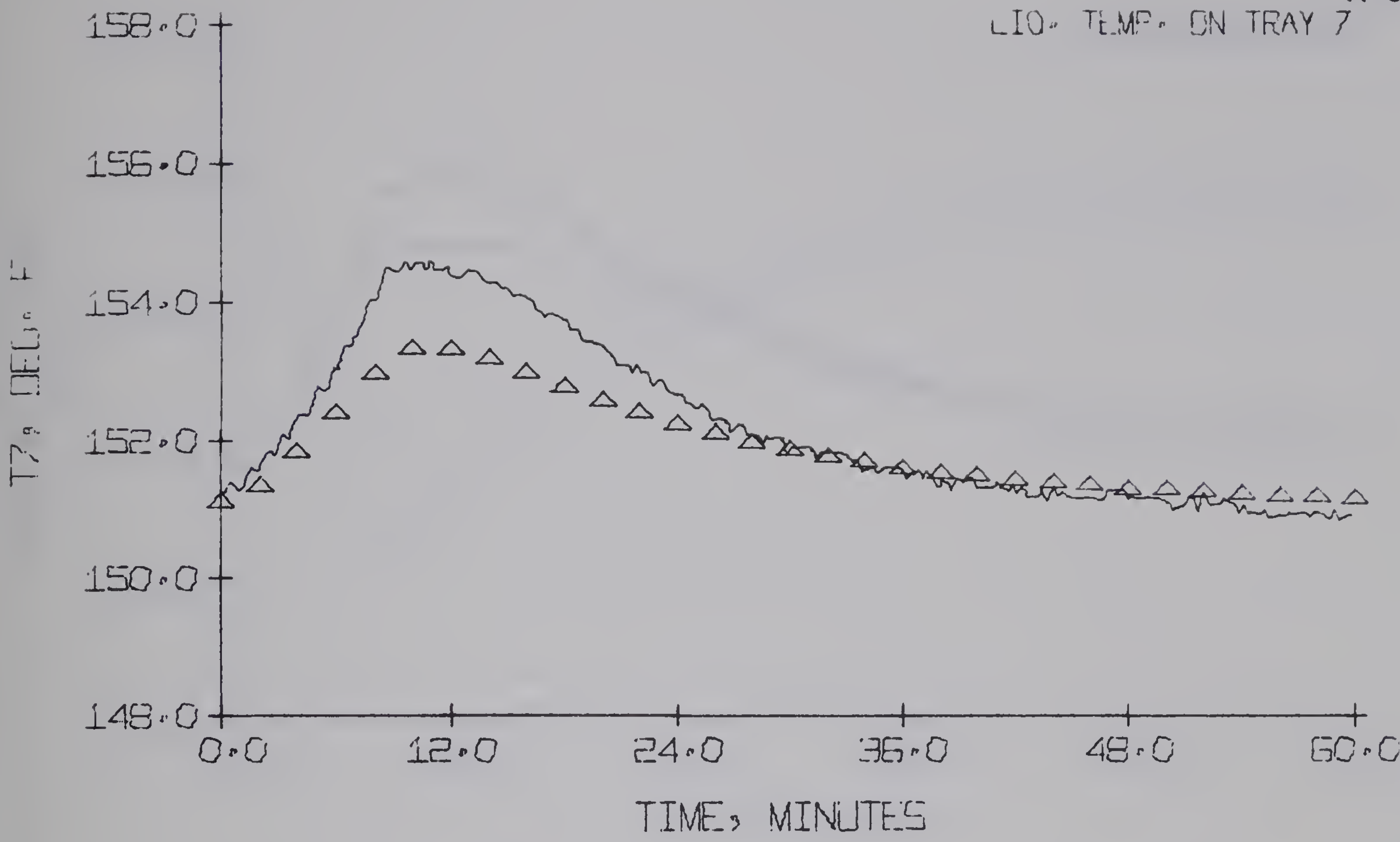

Figure A.2-49

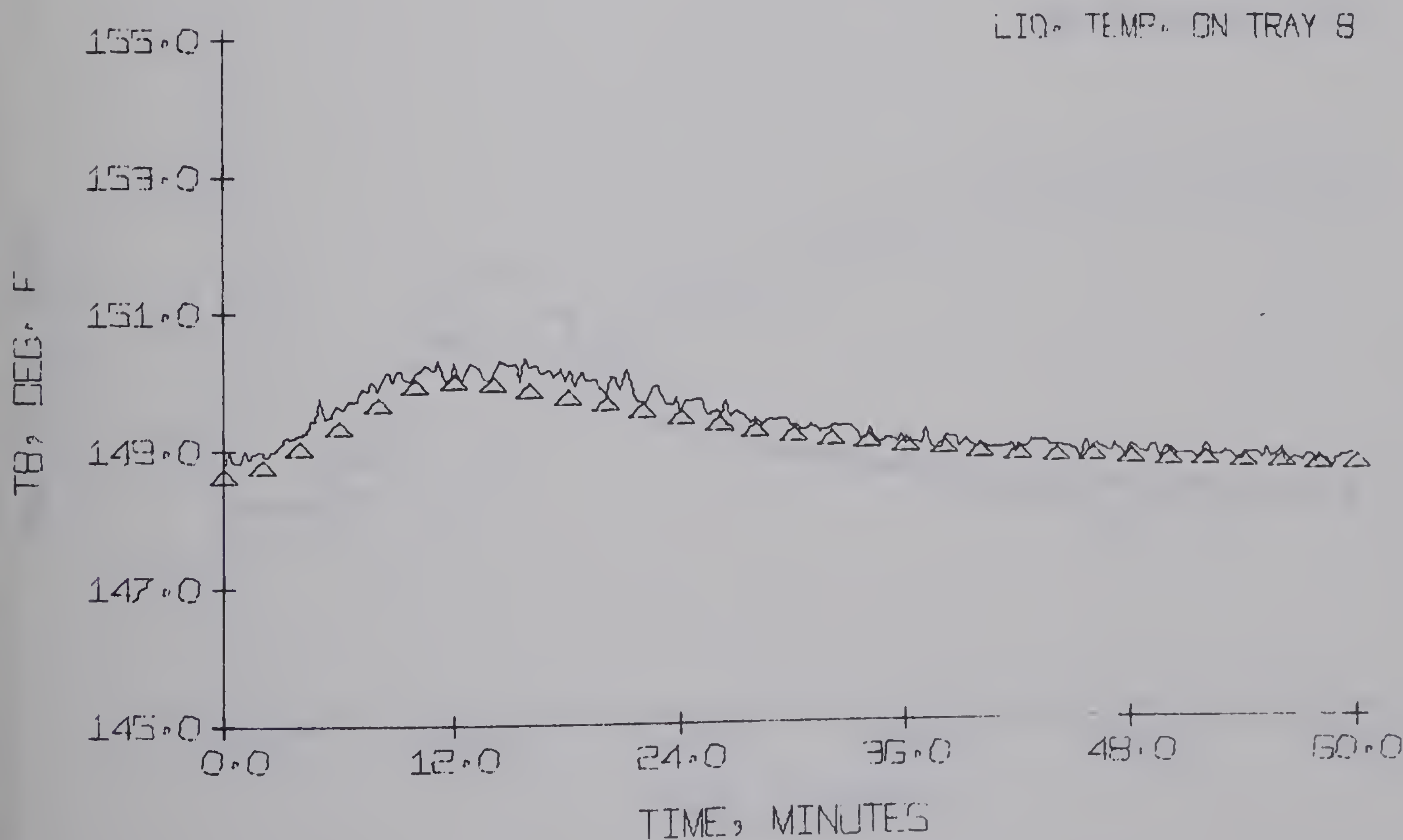

Figure A.2-50

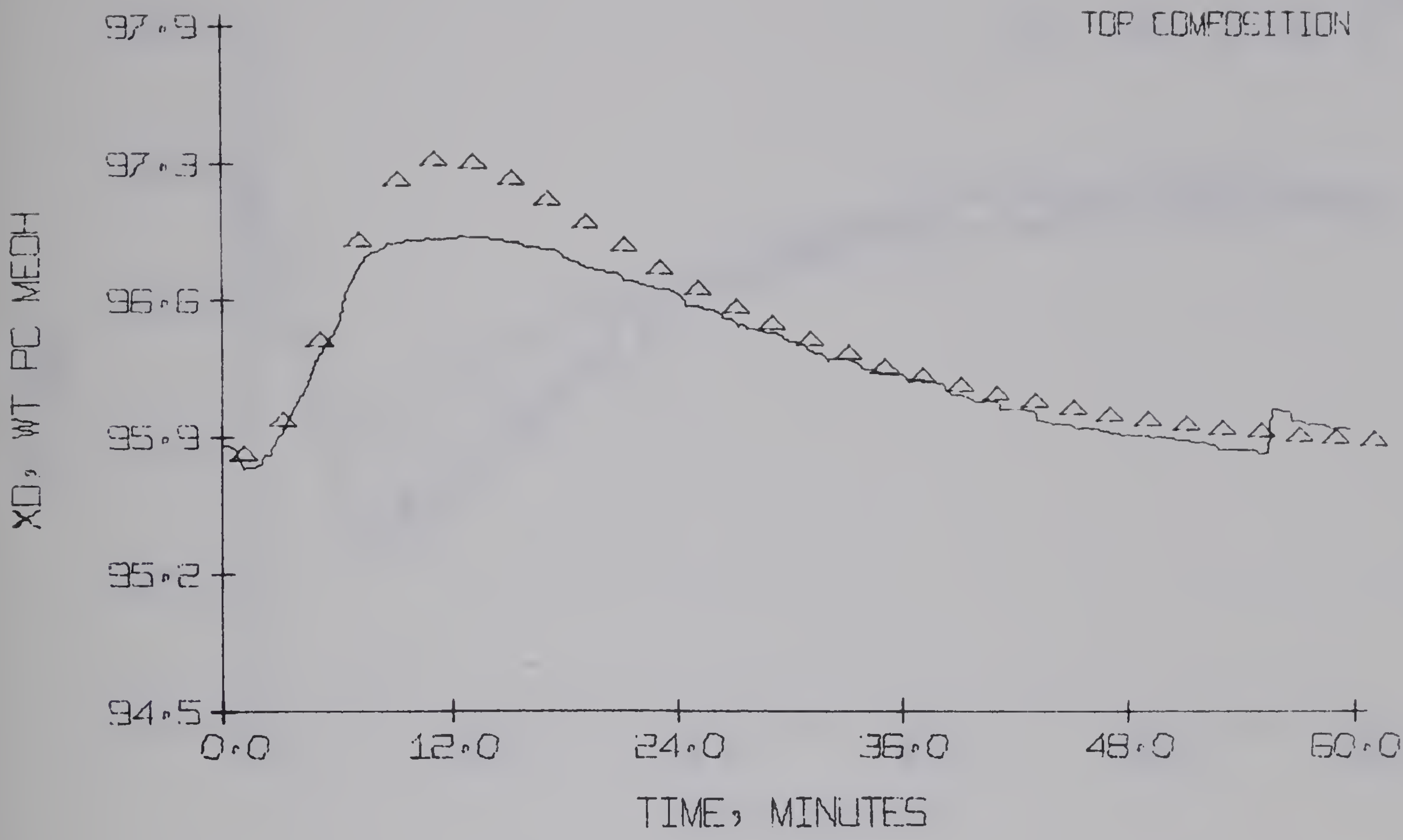

Figure A.2-51

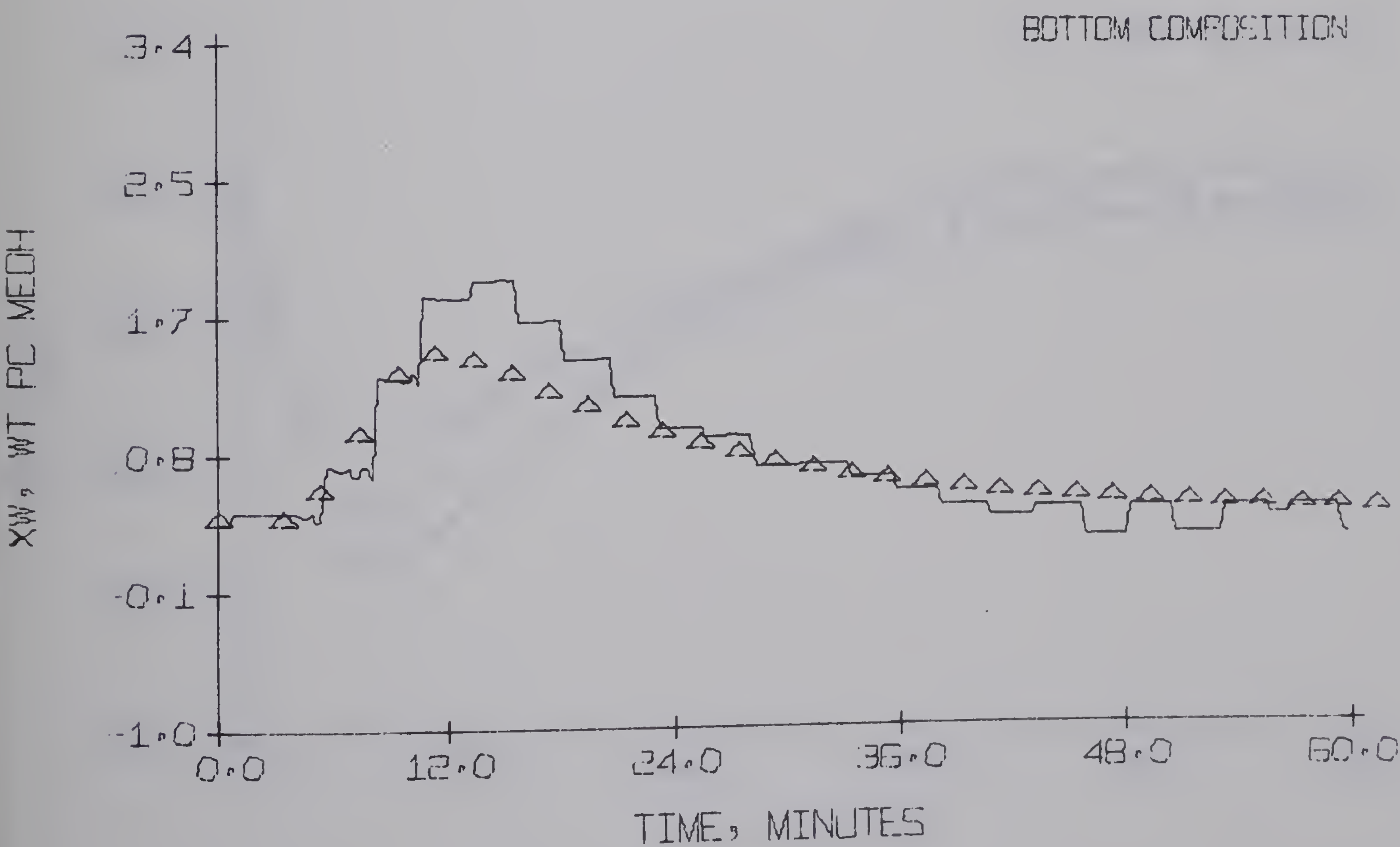

Figure A.2-52

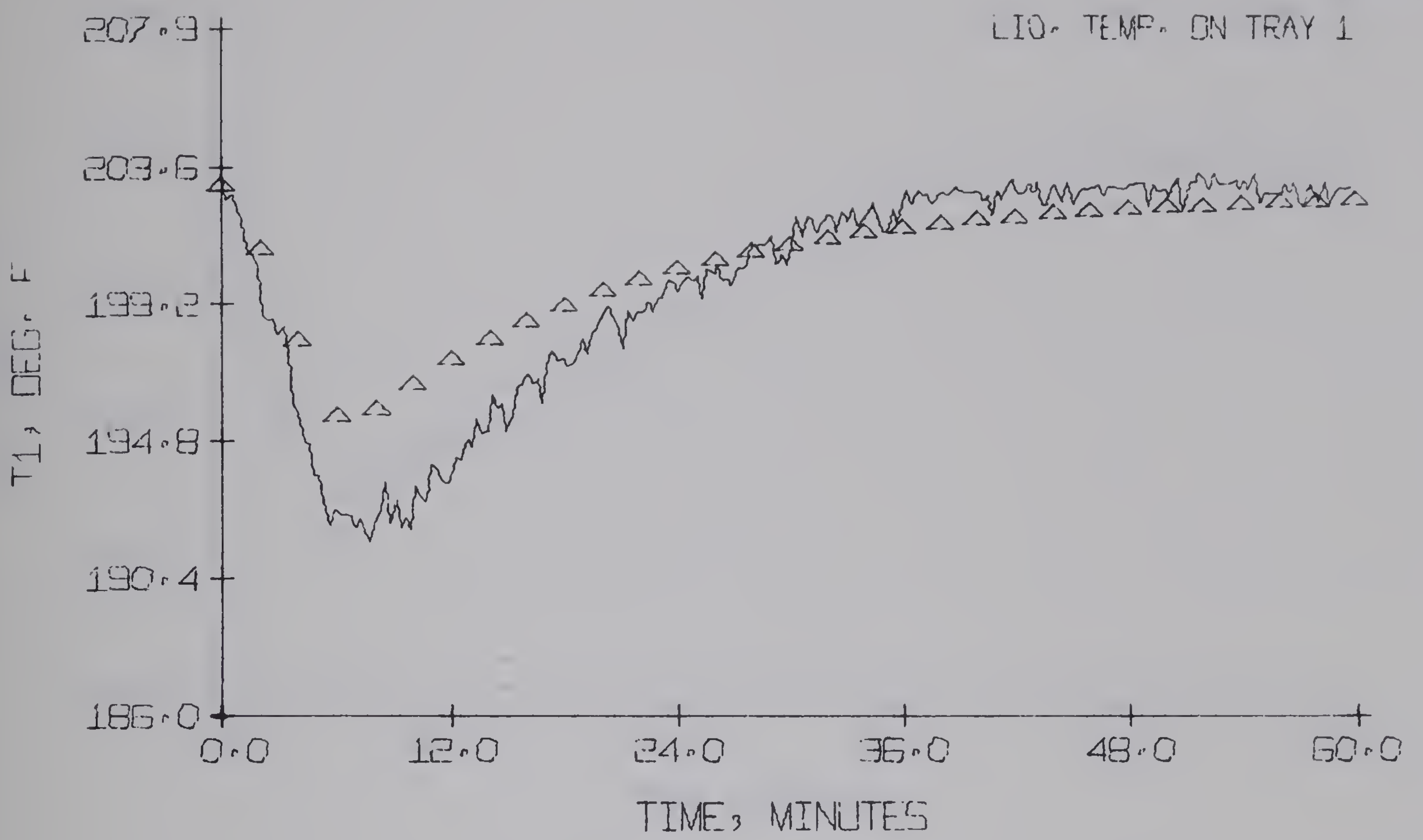

Figure A.2-53

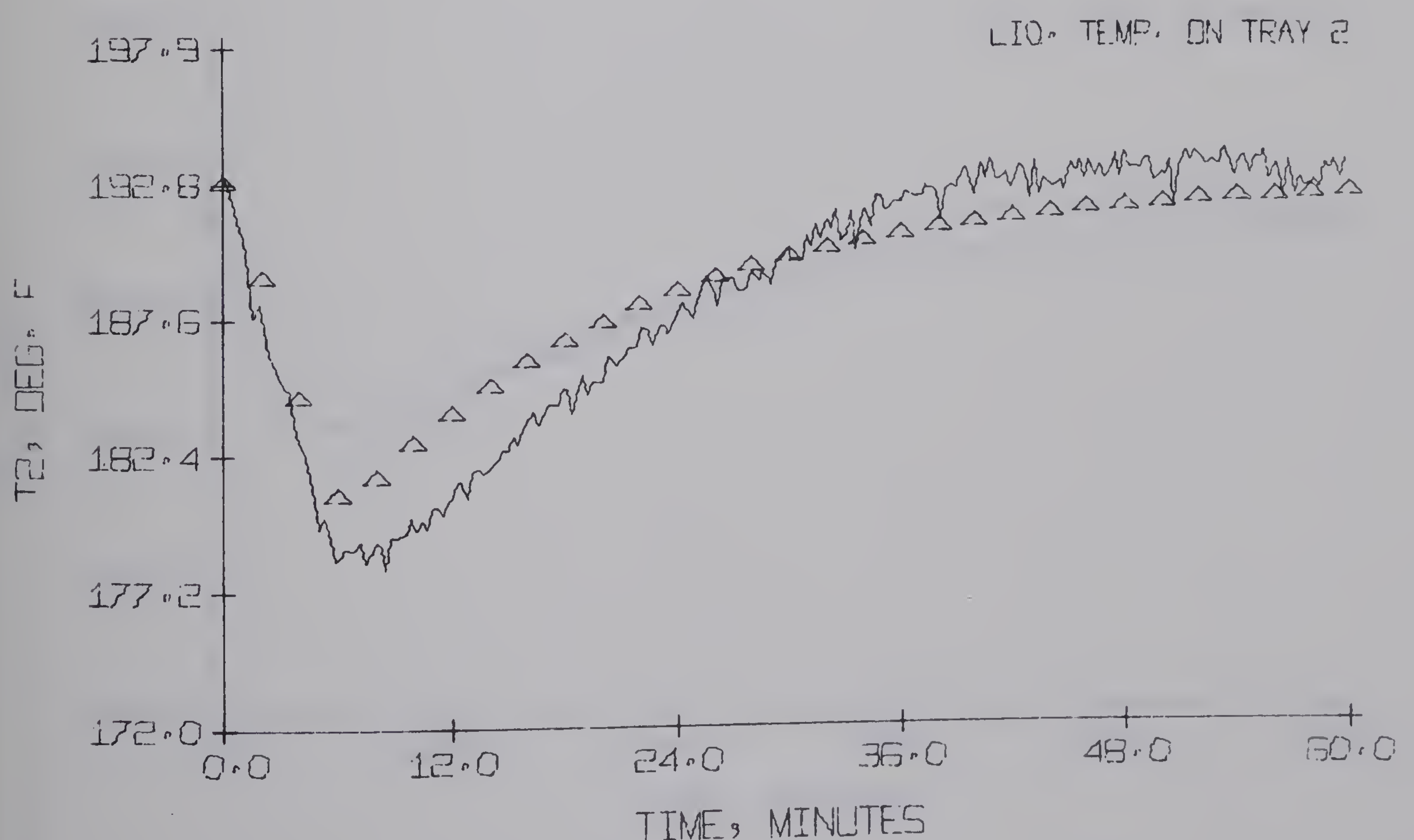

Figure A.2-54

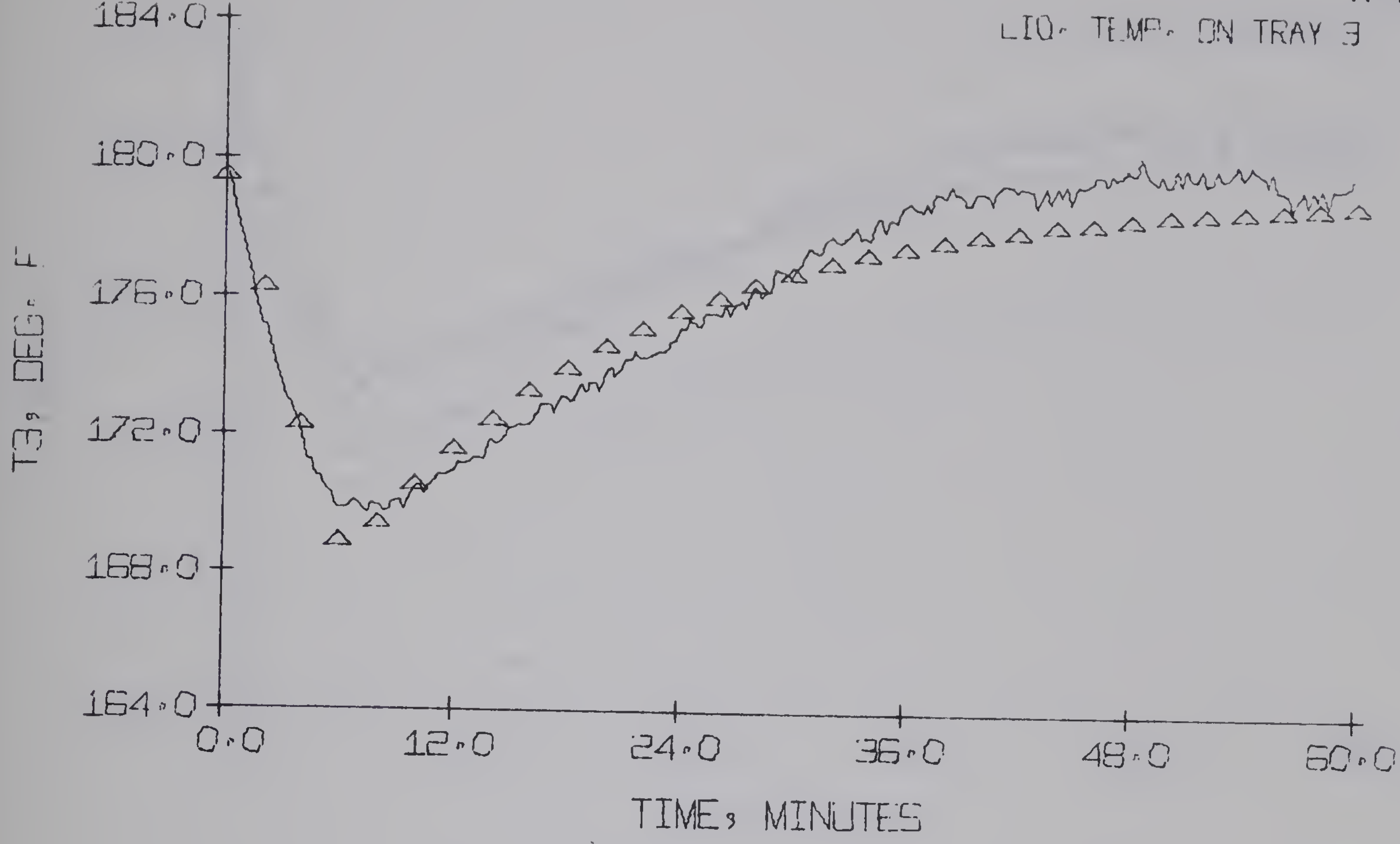

Figure A.2-55

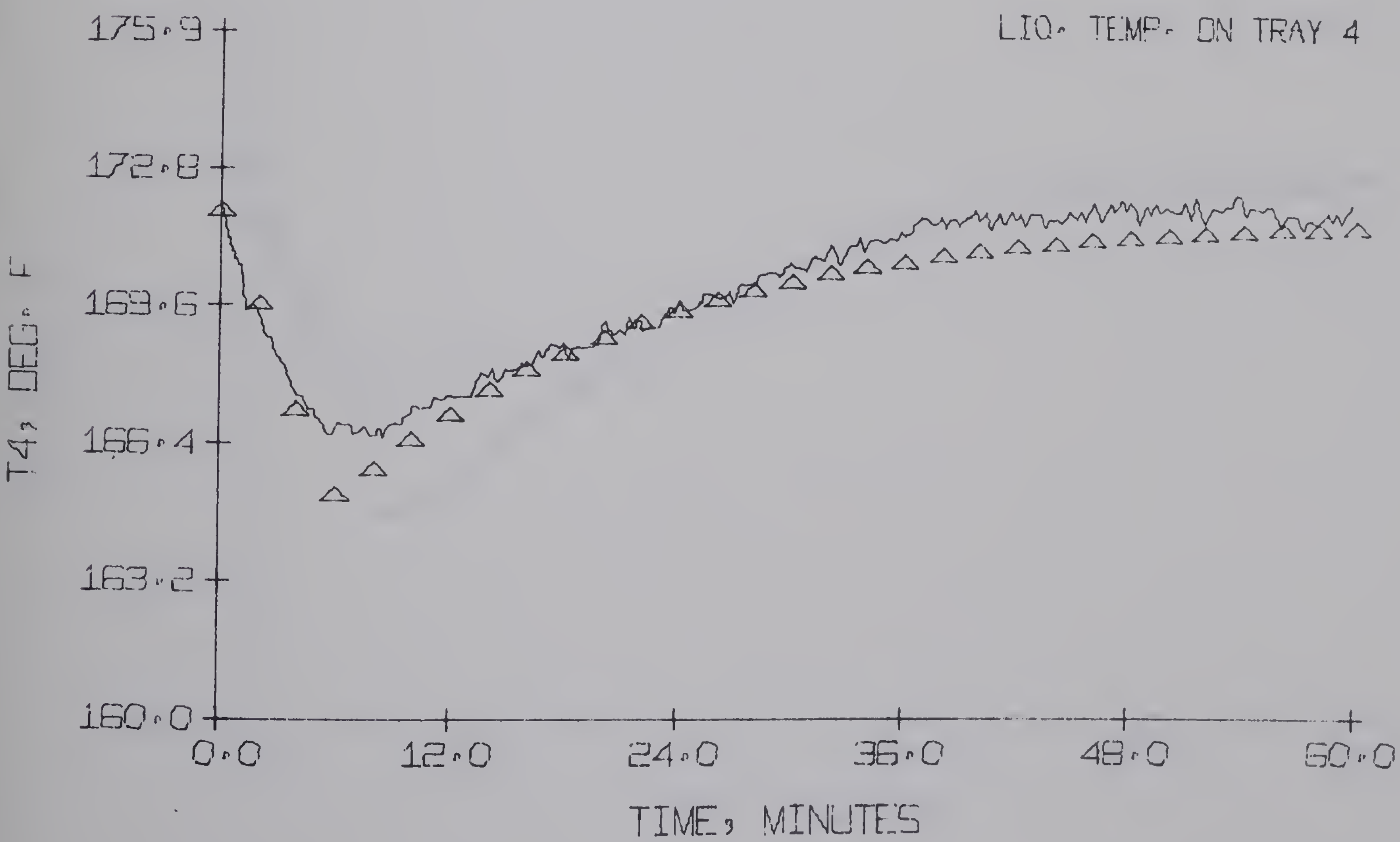

Figure A.2-56

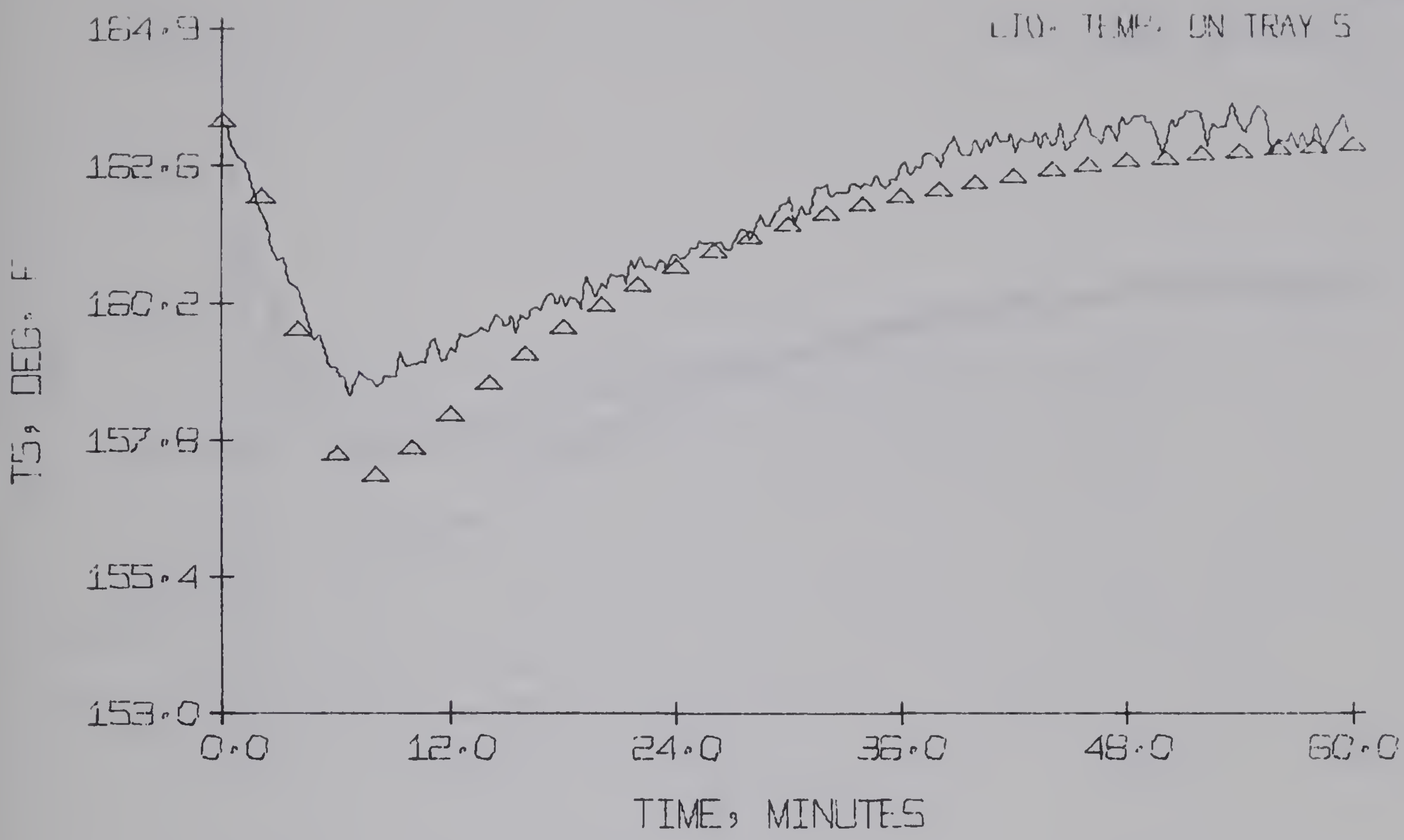

Figure A.2-57

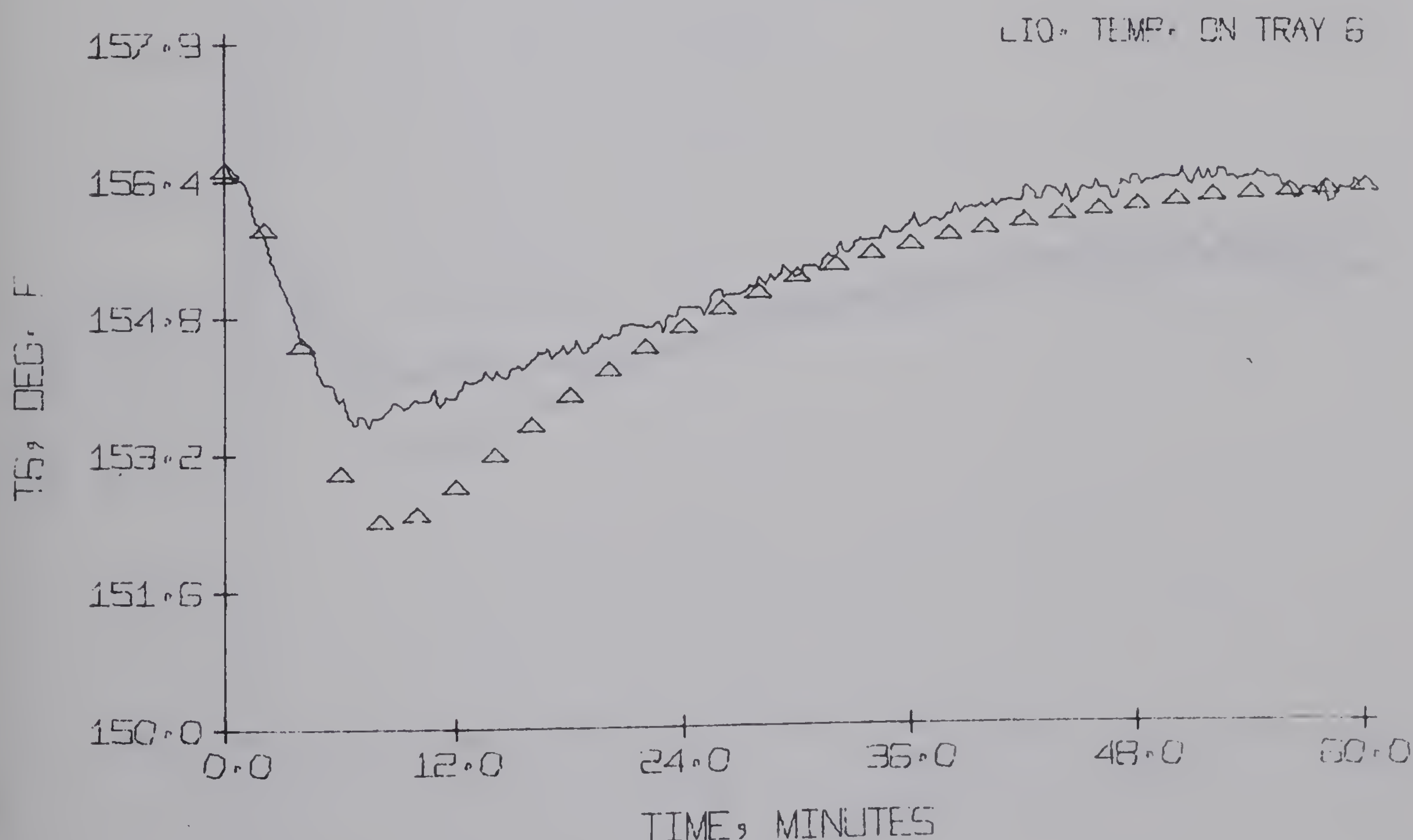

Figure A.2-58

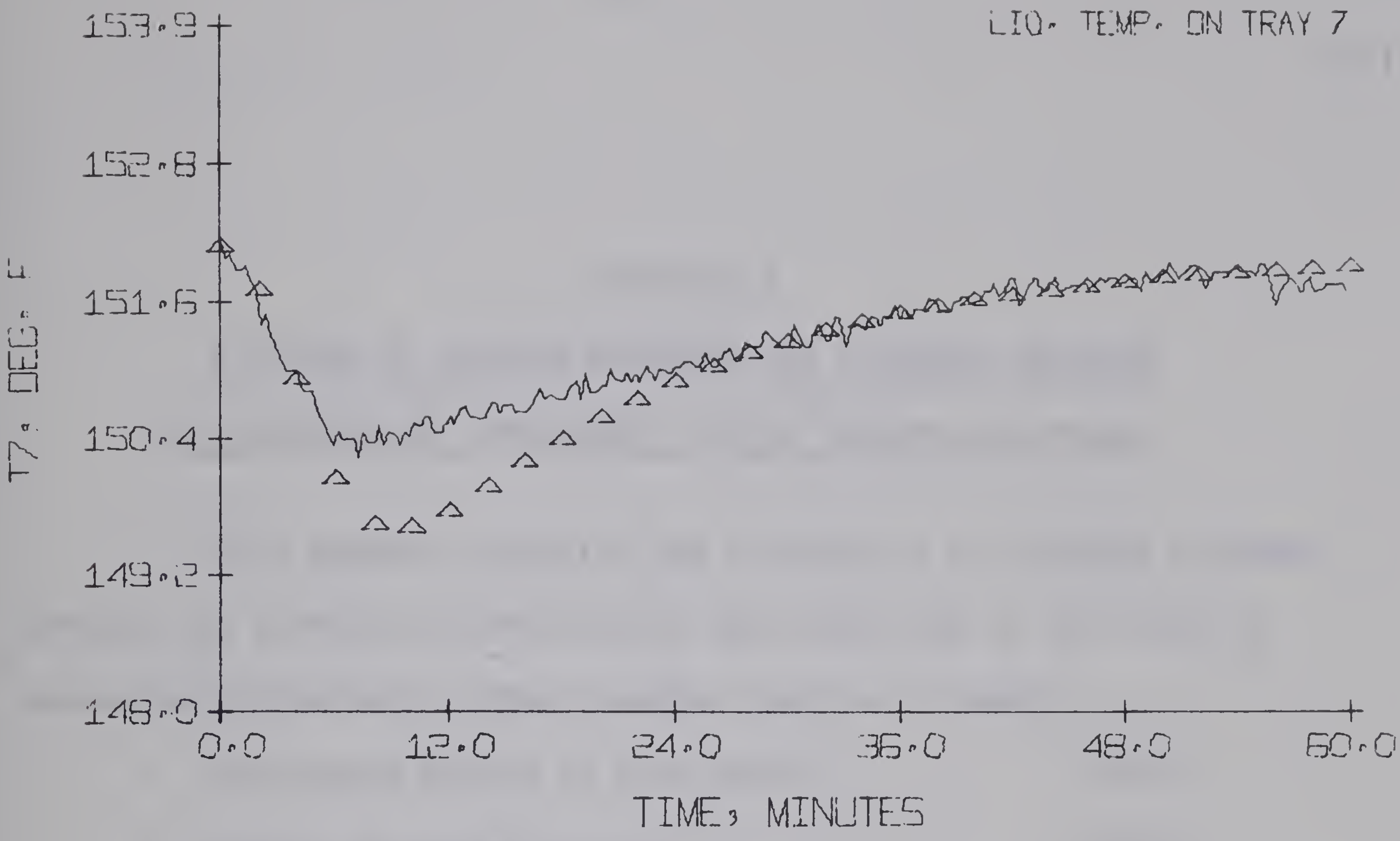

Figure A.2-59

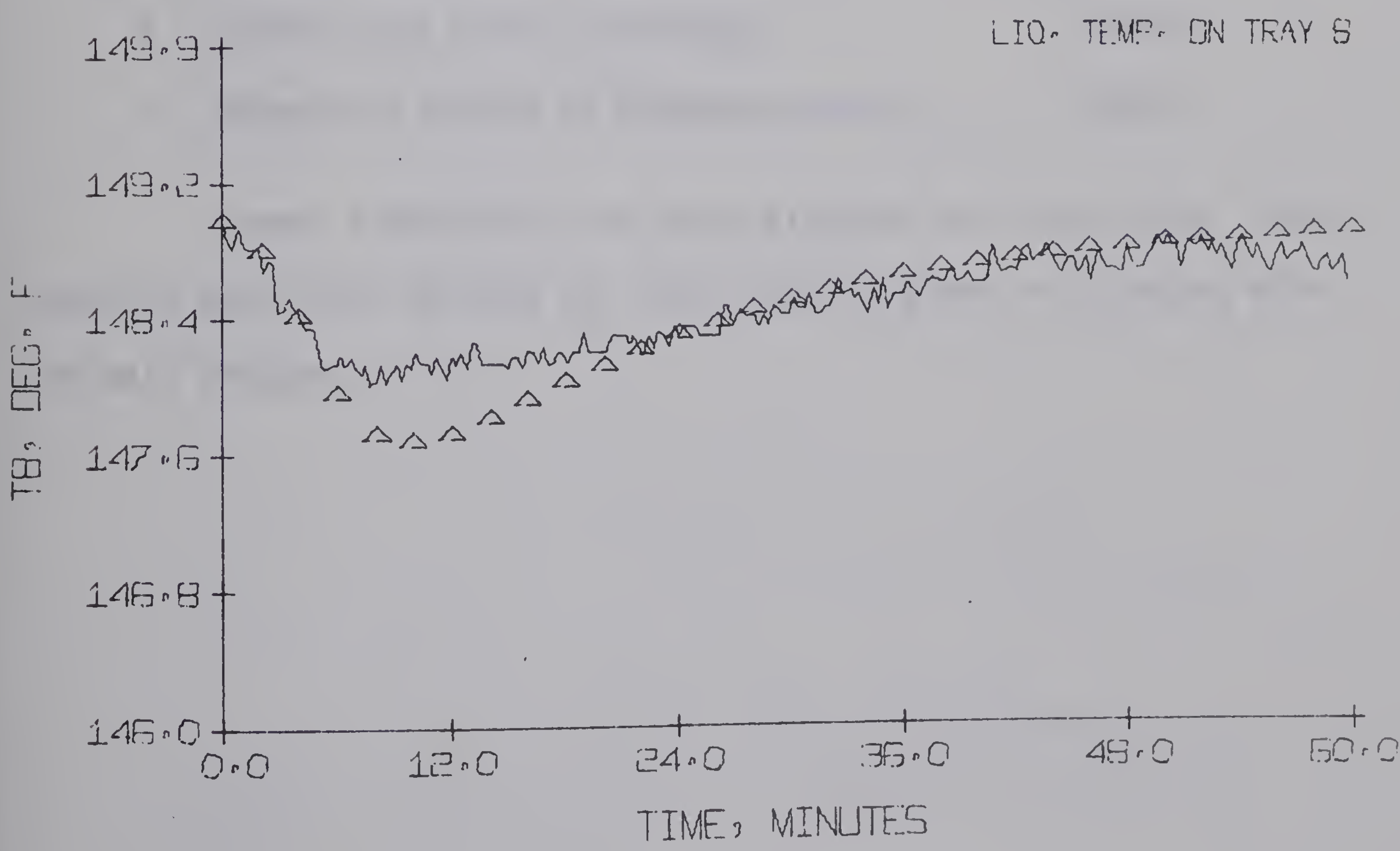

Figure A.2-60

APPENDIX B

LISTINGS OF FORTRAN PROGRAMS FOR DIFFERENT METHODS OF DETERMINING APPROXIMATE SYSTEM TRANSFER FUNCTIONS

This appendix contains the listings of all FORTRAN programs written for different methods which have been used in this work to determine approximate system transfer functions, namely:

1. Rosenbrock Method in Time-Domain (TDROO)
2. Bailey and Law Technique (FDBLO)
3. Chen and Philip Technique (FDCPO)
4. Levy Technique (FDLOO)
5. Staffin and Staffin Technique (FDSSO)
6. Rosenbrock Method in Frequency-Domain (FDROO)

Common subroutines for these programs are listed once. Subroutines especially written for individual programs are attached with the main program.

MAINLINE TDR00

```
      MAINLINE  TDR00
C
C
C           ****************************
C           *                          *
C           *    MAINLINE  TDR00       *
C           *    ---------------       *
C           *                          *
C           ****************************
C
C
C     PURPOSE
C        FIT THE TIME-DOMAIN DATA BY SIMPLE TRANSFER
C        FUNCTIONS USING ROSENBROCK'S SEARCH TECHNIQUES
C
C     DESCRIPTION OF PARAMETERS
C        NVAR      NUMBER OF PARAMETERS TO BE OPTIMIZED
C        M         PROGRAM CONTROL FLAG
C                   1 ... MAXIMIZE A FUNCTION
C                  -1 ... MINIMIZE A FUNCTION
C        CONVC     BASE POINT CONVERGENCE RATIO
C        ACONS     LOWER LIMITS FOR THE PARAMETERS
C        UCONS     UPPER LIMITS FOR THE PARAMETERS
C        B1        STARTING POINT
C        STEPS     INITIAL STEP SIZE FOR THE PARAMETERS
C        NCASE     NUMBER OF SETS OF DATA
C        WIDTH     PULSE WIDTH (MIN.)
C        HIGHT     PULSE HEIGHT
C        NWIDE     NUMBER OF DATA POINTS UNDER PULSE
C        NUMBR     NUMBER OF TRANSIENT RESPONSES IN EACH SET
C                  OF DATA
C        NPTS      NUMBER OF DATA POINTS
C        NSSPT     NUMBER OF STEADY-STATE DATA POINTS
C        Y         VECTOR OF INPUT DATA
C        ITYPE     CONTROL FLAG FOR THE TRANSFER FUNCTION
C                  GAIN
C                   1 ... POSITIVE GAIN
C                  -1 ... NEGATIVE GAIN
C        INDEX     CONTROL FLAG FOR THE TIME DELAY
C                   1 ... CALCULATE THE TIME DELAY
C                  -1 ... DO NOT CALCULATE THE TIME DELAY
C        ICONT     CONTROL FLAG FOR CALCULATIONS OF THE PULSE
C                  HEIGHT AND WIDTH
C                   1 ... CALCULATIONS REQUIRED
C                  -1 ... CALCULATIONS NOT REQUIRED
C        NRPLS     COLUMN NUMBER FOR THE FORCING FUNCTION
C        FLTCS     FILTER CONSTANT TO SMOOTH THE DATA
C        DEAD      TIME DELAY
C        DELT      SAMPLING TIME (MIN.)
```

MAINLINE TDROO ...(CONT'D)

```
C       USAGE
C          ENTER DATA AS REQUIRED
C
C       SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C          RBRCK, ADVCE, CONTR, DEDTM, SOLNS, FUNC
C
C

        DIMENSION STEPI(5)
        DIMENSION UCONI(5),ACONI(5)
        DIMENSION DATP(400,10),TITLE(20)
        DIMENSION DEAD(10),GAIN(10),TAU1(10),TAU2(10)
        COMMON AXES(5,5),B1(5),B2(5),UCONS(5),ACONS(5),A(5,5)
       *,B(5),
       1STEPS(5),BASE,BNEW,SUM,CONVC,AM(5),AJUMP,IFL(5),NVAR,M
       *,SNEW
        COMMON/ALEAS/Y(400),HIGHT,WIDTH,DELT,INDIC,NPTS,ITYPE
       *,SUMSQ
       1, NWIDE,NSSPT
        COMMON/TIMED/TDLAY
        DELT = 0.26666667
        READ (5,1) NVAR,M
      1 FORMAT (2I5)
        READ (5,3) CONVC
      3 FORMAT (F10.8)
        READ (5,2) (B1(I),I=1,5)
      2 FORMAT (5F10.5)
        READ (5,4) (ACONI(I),I=1,5)
        READ (5,4) (UCONI(I),I=1,5)
        READ (5,4) (STEPI(I),I=1,5)
      4 FORMAT (5F10.3)


        READ (5,10) NCASE
     10 FORMAT (I5)
        DO 9999  ICASE=1,NCASE
        READ (5,11) WIDTH,HIGHT,NWIDE
     11 FORMAT (2F10.3,I5)
        READ (5,12) NUMBR,NPTS,NSSPT,ITYPE,INDEX,ICONT,NRPLS
     12 FORMAT (7I5)
        READ (5,14) (DEAD(I),I=1,NUMBR)
     14 FORMAT (5F10.3)
        READ (5,15) FLTCS
     15 FORMAT (F10.3)


        WRITE (6,50)
     50 FORMAT(1H1,20X,'ROSENBROCK S SEARCH TECHNIQUE'/21X,'--
       *------------
       1---------------'//)
```

MAINLINE TDROO ...(CONT'D)

```
      WRITE (6,51) NVAR
   51 FORMAT (1H0,10X,'DIMENSIONS OF SPACE ',I3)
      WRITE (6,52) M
   52 FORMAT (1H0,10X,'CRITERION - MAXIMIZE (+1) , MINIMIZE
     * (-1)',I5)
      WRITE (6,53) CONVC
   53 FORMAT (1H0,10X,'BASE POINT CONVERGENCE RATIO',F14.8)
      WRITE (6,54)
   54 FORMAT (///11X,'INITIAL BASE POINT')
      WRITE (6,55) (B1(I),I=1,NVAR)
      WRITE (6,56)
   56 FORMAT (///11X, 'BASIC STEP SIZES')
      WRITE (6,55) (STEPI(I),I=1,NVAR)
      WRITE (6,57)
   57 FORMAT (///11X,'UPPER CONSTRAINTS')
      WRITE (6,55) (UCONI(I),I=1,NVAR)
      WRITE (6,58)
   58 FORMAT (///11X,'LOWER CONSTRAINTS')
      WRITE (6,55) (ACONI(I),I=1,NVAR)
   55 FORMAT (15X,F12.5)
      WRITE (6,70)
   70 FORMAT (1H1)


      READ (5,16) (TITLE(J),J=1,20)
   16 FORMAT (20A4)
      DO 1000  I=1,NPTS
      READ (5,100) (DATP(I,J),J=1,NUMBR)
  100 FORMAT (10F8.3)
 1000 CONTINUE
      IF(ICONT) 1010,1100,9999
 1010 CONTINUE

C         COMPUTE PULSE HEIGHT AND WIDTH

      WIDTH = NWIDE*DELT


      IBGIN = NSSPT+1
      IENDT = IBGIN+NWIDE
      SUMS = 0.0
      DO 1074  I=1,NSSPT
      SUMS = SUMS+DATP(I,NRPLS)
 1074 CONTINUE
      SSVAL = SUMS/FLOAT(NSSPT)
      SUMH = 0.0
      DO 1030  I=IBGIN,IENDT
      SUMH = SUMH+DATP(I,NRPLS)
 1030 CONTINUE
      SUMH = SUMH/(NWIDE+1)
```

MAINLINE TDROO ...(CONT'D)

```
      HIGHT = SUMH-SSVAL
      WRITE (6,981) HIGHT,WIDTH
  981 FORMAT (///7X,'PULSE HEIGHT IS =',F10.3,5X,'PULSE
     * WIDTH IS =',F10.
     13)
 1100 CONTINUE

C        CALCULATE DEAD TIME , GAIN , TAU1 , TAU2 OF THE
C        TRANSFER FUNCTION

      DO 4000  NUMB=1,NUMBR
      DO 3841  I=1,NVAR
      STEPS(I) = STEPI(I)
 3841 CONTINUE
      DO 5723  I=1,NVAR
      UCONS(I) = UCONI(I)
 5723 CONTINUE
      DO 5727  I=1,NVAR
      ACONS(I) = ACONI(I)
 5727 CONTINUE
      IF(NUMB-3) 3374,3373,3374
 3373 CONTINUE
      ITYPE = -ITYPE
 3374 CONTINUE

C        NO CALCULATION FOR THE FORCING FUNCTION

      IF(NUMB-NRPLS) 3500,4000,3500
 3500 CONTINUE
      DO 3510  I=1,NPTS
      Y(I) = DATP(I,NUMB)
 3510 CONTINUE

C        CALCULATE STEADY STATE VALUE

      SUMSS = 0.0
      DO 3550  K=1,NSSPT
      SUMSS = SUMSS+Y(K)
 3550 CONTINUE
      SSVAL = SUMSS/FLOAT(NSSPT)

C        SUBSTRACT OUT STEADY STATE VALUE

      DO 3560  K=1,NPTS
      Y(K) = Y(K)-SSVAL
 3560 CONTINUE

C        REDUCE NOISE EFFECT - USE FILTER CONSTANT TO SMOOTH
C        THE RESPONSE
```

MAINLINE TDROO ...(CONT'D)

```
      FILTR = 1.0-FLTCS
      DO 3540  I=2,NPTS
      Y(I) = FLTCS*Y(I-1)+FILTR*Y(I)
 3540 CONTINUE
      WRITE (6,34)
   34 FORMAT (///30X,'**** RESPONSE ****'/)
      WRITE (6,35) (Y(K),K=1,NPTS)
   35 FORMAT (4X,9F8.3)
      WRITE (6,36) SSVAL
   36 FORMAT (//21X,'INITIAL STEADY STATE VALUE IS',F10.4//)

C        IF INDEX EQUAL TO ZERO , NO CALCULATION OF THE TIME
C        DELAY

      IF(INDEX) 3530,3530,3520
 3520 CONTINUE

C        CALCULATE THE TIME DELAY USING SUBROUTINE DEDTM

      CALL DEDTM
      DEAD (NUMB) = TDLAY
 3530 CONTINUE
      NDELY = DEAD(NUMB)/DELT

C        COMPUTE THE GAIN AND TIME CONSTANTS FOR THE
C        TRANSFER FUNCTION

      INDIC = NSSPT+NDELY
      CALL RBRCK
      GAIN(NUMB) = B2(1)
      TAU1(NUMB) = B2(2)
      TAU2(NUMB) = B2(3)
 4000 CONTINUE
      WRITE (6,60) (TITLE(I),I=1,20)
   60 FORMAT (1H1///20A4)
      WRITE (6,61)
   61 FORMAT (///27X,'PROCESS PARAMETERS'/27X,'-------------
     *-----'//)
      WRITE (6,62)
   62 FORMAT (1H0,19X,'TIME DELAY',8X,'GAIN',11X,'TAU1',10X
     *,'TAU2'//)
      DO 65  I=2,NUMBR
      J = I-2
      WRITE (6,63) J,DEAD(I),GAIN(I),TAU1(I),TAU2(I)
   63 FORMAT (1H0,7X,'PLATE',I3,4F14.6)
   65 CONTINUE
 9999 CONTINUE
      STOP
      END
```

SUBROUTINE DEDTM

```
      SUBROUTINE DEDTM
C
C
C                   SUBROUTINE  DEDTM
C                   -----------------
C
C
C     PURPOSE
C        DETERMINE THE TIME DELAY OF ANY SYSTEM FROM ITS
C        TRANSIENT RESPONSE BY OLDENBOURG AND SARTORIUS'
C        METHOD
C
C     USAGE
C        CALL DEDTM
C
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C        NONE
C
C     REFERENCE
C        OLDENBOURG, R.C., AND SARTORIUS, H., 'THE DYNAMICS
C        OF AUTOMATIC CONTROL', AMERICAN SOCIETY OF
C        MECHANICAL ENGINEERS, NEW YORK, (1948)
C
C

      COMMON/ALEAS/Y(400),HIGHT,WIDTH,DELT,INDIC,NPTS,ITYPE
     *,SUMSQ
     1, NWIDE,NSSPT
      COMMON/TIMED/TDLAY

C        EVALUATE MAXIMUM DERIVATIVE OF THE RESPONSE

      NDUM = NWIDE/2
      IEND = NWIDE+NSSPT+NDUM+1
      DESAV = 0.0


      IBGIN = NSSPT+1
      DO 1202  I=IBGIN,IEND
      DERI  = 3.0*(Y(I+3)-Y(I-3))+2.0*(Y(I+2)-Y(I-2))+Y(I+1)
     *-Y(I-1)
      IF (ITYPE) 1204,1204,1203
 1203 CONTINUE
      IF(DERI-DESAV) 1202,1202,1205
 1204 CONTINUE
      IF(DERI-DESAV) 1205,1205,1202
 1205 CONTINUE
      IMAX = I
      DESAV = DERI
```

SUBROUTINE DEDTM ...(CONT'D)

```
 1202 CONTINUE
      WRITE (6,15) IMAX,Y(IMAX)
   15 FORMAT (1H0,10X,'MAXIMUM DERIVATIVE AT ',I5,'  VALUE
     * IS ',F14.5)
C          CALCULATE TIME DELAY

      AMAXD = DESAV/28.0
      ATST = Y(IMAX)/AMAXD+0.50
      ITST = ATST
      JTST = IMAX-ITST
      DUMY = Y(JTST)+Y(JTST+1)+Y(JTST-1)
      DUMMI = DUMY/3.0
      DUVA = DUMMI*2.718
      ZDE = DUVA/AMAXD+0.50
      SAT = ZDE+ATST
      ISAT = SAT
      NDELY = IMAX-NSSPT-ISAT
      IF (NDELY) 1500,1500,1501
 1500 CONTINUE
      NDELY = 0
 1501 CONTINUE
      TDLAY = NDELY*DELT

      WRITE (6,20) TDLAY
   20 FORMAT (1H0,10X,'TIME DELAY IS = ',F15.4)
      RETURN
      END
```

SUBROUTINE RBRCK

```
      SUBROUTINE RBRCK
C
C
C                    SUBROUTINE  RBRCK
C                    -----------------
C
C
C     PURPOSE
C        OPTIMIZE A FUNCTION BY VARYING ITS PARAMETERS
C
C     USAGE
C        CALL RBRCK
C
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C        ADVCE, CONTR, SOLNS, FUNC
C
C     METHOD
C        ROSENBROCK'S HILL CLIMBING METHOD
C
C     REFERENCES
C        ROSENBROCK, H.H., AND STOREY, C., 'COMPUTATION
C        TECHNIQUES FOR CHEMICAL ENGINEERS', PERGAMON PRESS,
C        NEW YORK, (1966).
C        WILDE, D.J., 'OPTIMUM SEEKING METHODS', PRENTICE
C        HALL, NEW JERSEY, (1964).
C
C
      COMMON AXES(5,5),B1(5),B2(5),UCONS(5),ACONS(5),A(5,5)
     *,B(5),
     1STEPS(5),BASE,BNEW,SUM,CONVC,AM(5),AJUMP,IFL(5),NVAR,M
     *,SNEW
      KSTEP = 0
      KROTN = 0
      NSUCS = 0
      NFAIL = 0
      IJUMP = 0
      AJUMP = 1.0
C        SET UP ORTHOGONAL AXES
      DO 1000  I=1,NVAR
      DO 1000  J=1,NVAR
      AXES(I,J) = 0.0
 1000 CONTINUE
      DO 1001  I=1,NVAR
      AXES(I,I) = 1.0
 1001 CONTINUE
```

SUBROUTINE RBRCK ...(CONT'D)

```
C         STARTING POINT

      DO 1004  I=1,NVAR
      B2(I) = B1(I)
 1004 CONTINUE

C         EVALUATE THE FUNCTION AT THE BASE POINT

      BASE = FUNC(NVAR,B2)
      WRITE (6,100) BASE
  100 FORMAT (1H0,8X,'INITIAL BASE POINT'/12X,'INITIAL
     * FUNCTION VALUE IS
     1',E16.8//)
      CONVC = CONVC*16.0


 1002 CONTINUE
      BNEW = BASE
 1999 CONTINUE
      DO 1003  I=1,NVAR
      AM(I) = 3.0
      IFL(I) = 0
 1003 CONTINUE
      DO 1007  K=1,NVAR
      CALL ADVCE(K)
      CALL CONTR
      KSTEP = KSTEP+1
      SNEW = FUNC(NVAR,B2)
      WRITE (6,101) KROTN,KSTEP,B2(1),B2(2),B2(3),SNEW
      IF(M*(BNEW-SNEW)) 1005,1006,1006

C         SUCCESS

 1005 CONTINUE
      BNEW = SNEW
      GO TO 1007

C         FAILURE

 1006 AM(K) = -AM(K)
      CALL ADVCE(K)
      KSTEP = KSTEP+1
 1007 CONTINUE
 1020 CONTINUE

C         SET CHECK VALUE TO ZERO FOR JUMP CONVERGENCE

      ICHEK = 0

C         GO ON UNTIL AT LEAST ONE TRIAL HAD BEEN SUCCESSFUL
```

SUBROUTINE RBRCK ...(CONT'D)

```
C           IN EACH DIRECTION AND ONE HAD FAILED
      DO 2020  K=1,NVAR
C           CHECK WHETHER THE INCREASE INSTEP SIZE IS TWO SMALL
      IF(ABS(AM(K))-0.80) 2001,2002,2002
 2001 CONTINUE
      ICHEK = ICHEK+1
      GO TO 2020
 2002 CONTINUE
      CALL ADVCE(K)
      CALL CONTR
      KSTEP = KSTEP+1
      SNEW = FUNC(NVAR,B2)
      WRITE (6,101) KROTN,KSTEP,B2(1),B2(2),B2(3),SNEW
  101 FORMAT (7X,2I8,4E15.5)
C           CHECK IF THE NEW TRIAL IS SUCCESSFUL
      IF(M*(BNEW-SNEW)) 2003,2010,2010
 2003 CONTINUE
C           SUCCESSFUL - TREBLE STEP SIZE
      IF( ABS(BNEW-SNEW)-3.0*CONVC) 2009,2004,2004
 2004 CONTINUE
      IF(IFL(K)) 2005,2005,2006
 2005 CONTINUE
      AM(K) = 3.0*AM(K)
 2006 CONTINUE
      BNEW = SNEW
      GO TO 2015
 2009 CONTINUE
      AM(K) = 0.50*AM(K)
      BNEW = SNEW
      GO TO 2015
 2010 CONTINUE
C           FAILURE - MULTIPLY STEP SIZE BY -0.50
      AM(K) = -AM(K)
      CALL ADVCE(K)
      AM(K) = 0.50*AM(K)
      IFL(K) = 1
 2015 CONTINUE
C           CHECK WHETHER STEP SIZE IS TOO LARGE
```

SUBROUTINE RBRCK ...(CONT'D)

```
      IF(ABS(AM(K))-18.0) 2020,2020,2016
 2016 CONTINUE
      AM(K) = 18.0*AM(K)/ABS(AM(K))
 2020 CONTINUE
      IF(ICHEK-NVAR) 1020,2500,2500

C         CHECK WHETHER PROGRESS HAD BEEN MADE OR NOT

 2500 CONTINUE
      IF(M*(BASE-BNEW)) 2510,2501,2503
 2501 CONTINUE

C         NO PROGRESS WHATSOEVER

      IJUMP = IJUMP+1
      DO 2502 K=1,NVAR
      AM(K) = 1.50/IJUMP
      IFL(K) = 0
 2502 CONTINUE


      IF(IJUMP-2) 1003,1003,2520
 2503 CONTINUE
      NSUCS = NSUCS+1
      IJUMP = 0
      IF(NSUCS-2) 2504,2510,2510
 2504 CONTINUE
      GO TO 1999
 2510 CONTINUE
      NSUCS = 0
      IJUMP = 0
      IF(M*(BASE-BNEW)+CONVC) 4010,2506,2506
 2506 CONTINUE
      NFAIL = NFAIL+1
      WRITE (6,200) NFAIL
  200 FORMAT (1H0,8X,'****INSIGNIFICANT MOVE - NFAIL IS'I3,'
     *****')
      IF(NFAIL-2) 4020,2520,2520
 2520 CONTINUE

C         REDUCE INITIAL STEP SIZE BY HALF AND TRY AGAIN FROM
C         THE INITIAL BASE POINT

      NFAIL = 0
      IJUMP = 0
      AJUMP = AJUMP/2.0
      CONVC = CONVC/2.0
      IF(AJUMP-0.050) 8000,8000,4000
 4000 CONTINUE
      BNEW = BASE
```

SUBROUTINE RBRCK ...(CONT'D)

```
      DO 4001  K=1,NVAR
      B2(I) = B1(I)
 4001 CONTINUE
      WRITE (6,400)
  400 FORMAT (1H0,8X,'****STEP SIZE HAS BEEN REDUCED BY HALF
     *****')
      GO TO 1002
 4010 CONTINUE
      NFAIL = 0
 4020 CONTINUE


      KROTN = KROTN+1

C         ROTATION OF AXES USING GRAM-SCHMIDT
C         ORTHOGONALIZATION PROCESS
C     REFERENCE - WILDE'S OPTIMUM SEEKING METHOD, PAGE 155
C
C
C         EQUATION 5-16A

      DO 8500  I=1,NVAR
      A(1,I) = B2(I)-B1(I)
 8500 CONTINUE

C         EQUATION 5-16C

      DO 8502  I=2,NVAR
      IM1 = I-1
      DO 8501  J=1,IM1
      A(I,J) = 0.0
 8501 CONTINUE
      DO 8502  J=I,NVAR
      A(I,J) = A(1,J)
 8502 CONTINUE

C         EQUATION 5-17

      SUMA = 0.0
      DO 8503  J=1,NVAR
      SUMA = SUMA+A(1,J)*A(1,J)
 8503 CONTINUE
      DO 8504  J=1,NVAR
      AXES(1,J) = A(1,J)/SQRT(SUMA)
 8504 CONTINUE

C         EQUATION 5-21

      DO 8508  I=2,NVAR
      SUMA = 0.0
```

SUBROUTINE RBRCK ...(CONT'D)

```
      DO 8505  J=1,NVAR
      SUMA = SUMA+AXES(I-1,J)*A(I,J)
 8505 CONTINUE
      DO 8506  J=1,NVAR
      B(J) = A(I,J)-AXES(I-1,J)*SUMA
 8506 CONTINUE


      SUMB = 0.0
      DO 8507  J=1,NVAR
      SUMB = SUMB+B(J)*B(J)
 8507 CONTINUE


      DO 8508  J=1,NVAR
      AXES(I,J) = B(J)/SQRT(SUMB)
 8508 CONTINUE

C        END OF THIS PART OF ROTATION OF AXES
C        REDEFINE BASE POINT

      BASE = BNEW
      DO 8100  K=1,NVAR
      B1(K) = B2(K)
 8100 CONTINUE
      GO TO 1002
 8000 CALL SOLNS(KROTN,KSTEP)
      RETURN
      END
```

SUBROUTINE ADVCE

```
      SUBROUTINE ADVCE(K)
C                    SUBROUTINE  ADVCE
C                    -----------------
C
C
C     PURPOSE
C        DETERMINE NEW VALUES FOR EACH VARIABLES
C
C     DESCRIPTION OF PARAMETERS
C        K          VARIABLE NUMBER
C
C     USAGE
C        CALL ADVCE (K)
C
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C        NONE
C
C
      COMMON AXES(5,5),B1(5),B2(5),UCONS(5),ACONS(5),A(5,5)
     *,B(5),
     1STEPS(5),BASE,BNEW,SUM,CONVC,AM(5),AJUMP,IFL(5),NVAR,M
     *,SNEW
      DO 100  I=1,NVAR
      B2(I) = B2(I)+STEPS(I)*AXES(I,K)*AM(K)*AJUMP
  100 CONTINUE
      RETURN
      END
```

SUBROUTINE CONTR

```
      SUBROUTINE CONTR
C
C
C                    SUBROUTINE  CONTR
C                    -----------------
C
C
C     PURPOSE
C        INSERT CONSTRAINTS ON THE PARAMETERS TO BE
C        OPTIMIZED
C
C     USAGE
C        CALL CONTR
C
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C        NONE
C
C     REFERENCE
C        ROSENBROCK, H.H., AND STOREY, C., 'COMPUTATION
C        TECHNIQUES FOR CHEMICAL ENGINEERS', PERGAMON PRESS,
C        NEW YORK, (1966).
C
C

      COMMON AXES(5,5),B1(5),B2(5),UCONS(5),ACONS(5),A(5,5)
     *,B(5),
     1STEPS(5),BASE,BNEW,SUM,CONVC,AM(5),AJUMP,IFL(5),NVAR,M
     *,SNEW
      ICHEK = 0


      DO 100  I=1,NVAR
      IF(B2(I)-UCONS(I)) 102,101,101
  101 CONTINUE
      B2(I) = UCONS(I)
      AM(I) = -0.50*AM(I)
      ICHEK = ICHEK+1
      GO TO 100
  102 CONTINUE


      IF(B2(I)-ACONS(I)) 103,103,100
  103 CONTINUE
      B2(I) = ACONS(I)
      AM(I) = -0.50*AM(I)
      ICHEK = ICHEK+1
  100 CONTINUE
      IF(ICHEK-NVAR) 104,105,105
  105 CONTINUE
```

SUBROUTINE CONTR ...(CONT'D)

```
      WRITE (6,110) KSTEP
  110 FORMAT (1H0,'*** ALL VARIABLES AT CONSTRAINTS AFTER
     * JUMP',I5/)
      BNEW = FUNC(NVAR,B2)
      CALL SOLNS(KROTN,KSTEP)
      STOP
  104 CONTINUE
      RETURN
      END
```

SUBROUTINE SOLNS

```
      SUBROUTINE SOLNS(KROTN,KSTEP)
C
C
C                   SUBROUTINE  SOLNS
C                   -----------------
C
C
C     PURPOSE
C        WRITE OUT THE FINAL POINT AND THE FINAL FUNCTION
C        VALUE
C
C     DESCRIPTION OF PARAMETERS
C        KROTN     NUMBER OF AXES OF ROTATION
C        KSTEP     NUMBER OF STEPS FORWARD
C
C     USAGE
C        CALL SOLNS (KROTN, KSTEP)
C
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C        NONE
C
C
      COMMON AXES(5,5),B1(5),B2(5),UCONS(5),ACONS(5),A(5,5)
     *,B(5),
     1STEPS(5),BASE,BNEW,SUM,CONVC,AM(5),AJUMP,IFL(5),NVAR,M
     *,SNEW
      WRITE (6,100)
  100 FORMAT(1H1,//30X,'ROSENBROCK S SEARCH TECHNIQUE'//)
      WRITE (6,110)
  110 FORMAT (1H0,10X,'CONVERGENCE CRITERION IS SATISFIED')


      WRITE (6,120) KROTN
  120 FORMAT (1H0,10X,I10,'  AXES OF ROTATION')
      WRITE (6,130) KSTEP
  130 FORMAT (1H0,10X,I10,'  STEPS FORWARD')
      WRITE (6,140)
  140 FORMAT (1H0,10X,'FINAL POINT IS ')
      WRITE (6,150) (B2(I),I=1,NVAR)
  150 FORMAT (1H0,10X,3E16.8)


      WRITE (6,160)
  160 FORMAT (1H0,10X,'FINAL FUNCTION VALUE')
      WRITE (6,170) BNEW
  170 FORMAT (1H0,15X,E16.8)
      WRITE (6,180)
  180 FORMAT (1H1)
```

SUBROUTINE SOLNS ...(CONT'D)

```
      RETURN
      END
```

FUNCTION FUNC

```
      FUNCTION FUNC(NVAR,B2)
C
C
C                     FUNCTION  FUNC
C                     --------------
C
C
C     PURPOSE
C        COMPUTE THE VALUE OF THE FUNCTION TO BE OPTIMIZED
C        THE MODEL IS THAT OF TWO FIRST ORDER TRANSFER
C        FUNCTIONS IN SERIES
C        FORCING FUNCTION  - RECTANGULAR PULSE
C
C     DESCRIPTION OF PARAMETERS
C        NVAR      NUMBER OF PARAMETERS TO BE OPTIMIZED
C        B2        VALUES OF THE RESPECTIVE PARAMETERS
C
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C        NONE
C
C
      COMMON/ALEAS/Y(400),HIGHT,WIDTH,DELT,INDIC,NPTS,ITYPE
     *,SUMSQ
     1, NWIDE,NSSPT
      DIMENSION B2(5)
      GAIN = B2(1)
      TAU1 = B2(2)
      TAU2 = B2(3)
      TIME = 0.0
      SUMSQ = 0.0
      DO 100  I=INDIC,NPTS
      IF(TIME-WIDTH) 250,250,251
  250 CONTINUE
      U = 0.0
      GO TO 252
  251 CONTINUE
      U = 1.0
  252 CONTINUE
      T2MT1 = TAU2-TAU1
      RAPT1 = TAU1/T2MT1
      RAPT2 = TAU2/T2MT1
      TIMA = TIME-WIDTH
      EXPRT = 1.0+RAPT1*EXP(-TIMA/TAU1)-RAPT2*EXP(-TIMA
     */TAU2)
      EXPRS = 1.0+RAPT1*EXP(-TIME/TAU1)-RAPT2*EXP(-TIME
     */TAU2)
     1-U*EXPRT
      AMODL = HIGHT*GAIN*EXPRS*ITYPE
```

FUNCTION FUNC ...(CONT'D)

```
      TIME = TIME+DELT
      SUMSQ = SUMSQ+(Y(I)-AMODL)**2
  100 CONTINUE
      FUNC = SUMSQ
      RETURN
      END
```

MAINLINE FDBLO

```
      MAINLINE FDBLO

C
C
C              *************************
C              *                       *
C              *   MAINLINE  FDBLO     *
C              *   ---------------     *
C              *                       *
C              *************************
C
C
C     PURPOSE
C        FITTING FREQUENCY-DOMAIN DATA BY FIRST, SECOND OR
C        THIRD ORDER TRANSFER FUNCTION
C
C     DESCRIPTION OF PARAMETERS
C        NCASE     NUMBER OF SETS OF DATA TO BE FITTED
C        IFLAG     PROGRAM CONTROL FLAG
C                   1 ... FIT THE DATA BY OVERDAMPED
C                  TRANSFER FUNCTIONS SUCH AS FIRST, SECOND
C                  OR THIRD ORDER
C                  -1 ... FIT THE DATA BY AN UNDERDAMPED
C                  SECOND ORDER TRANSFER FUNCTION
C        NFQ       NUMBER OF DATA POINTS
C        GAIN      GAIN OF THE TRANSFER FUNCTION
C        OMEGA     FREQUENCY
C        AMAT      MAGNITUDE OF THE BODE PLOT
C
C     USAGE
C        ENTER DATA AS REQUIRED
C
C     REMARKS
C        GAIN OF THE TRANSFER FUNCTION SHOULD BE KNOWN
C

      DIMENSION OMEGA(50),AMAG(50),AMAT(50)
      READ (5,1) NCASE
    1 FORMAT (I3)
      DO 1000 K=1,NCASE
      READ (5,1) IFLAG

C        READ IN DATA

      READ (5,2) NFQ, GAIN
    2 FORMAT (I5, F10.3)
      READ (5,3)  (OMEGA(IW),AMAT(IW),IW=1,NFQ)
    3 FORMAT (10X,F9.4,17X,F9.4)
      DO 333 KL=1,NFQ
      AMAG(KL) = AMAT(KL)/GAIN
```

MAINLINE FDBLO ...(CONT'D)

```
  333 CONTINUE
C         DETERMINE WHICH SUBROUTINE IS TO BE CALLED BL123
C         OR BLUND
C
      IF (IFLAG) 200,200,202
  200 CONTINUE
C         UNDERDAMPED - CALL BLUND
      CALL BLUND (OMEGA,AMAG,NFQ)
      GO TO 1000
  202 CONTINUE
C         OVERDAMPED - CALL BL123
      CALL BL123 (OMEGA,AMAG,NFQ)
 1000 CONTINUE
      STOP
      END
```

SUBROUTINE BL123

```
      SUBROUTINE BL123 (OMEGA,AMAG,NFQ)
C
C
C                    SUBROUTINE  BL123
C                    -----------------
C
C
C     PURPOSE
C        FIT THE FREQUENCY-DOMAIN DATA BY OVERDAMPED
C        TRANSFER FUNCTIONS SUCH AS FIRST, SECOND OR THIRD
C        ORDER
C
C     DESCRIPTION OF PARAMETERS
C        OMEGA    FREQUENCY
C        AMAG     AMPLITUDE RATIO
C        NFQ      NUMBER OF DATA POINTS
C
C     USAGE
C        CALL BL123 (OMEGA,AMAG,NFQ)
C
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C        SOLEQ
C
C     METHOD
C        BAILEY AND LAW'S NON LINEAR REGRESSION TECHNIQUE
C
C     REFERENCE
C        BAILEY, R.V., AND LAW, V.J., 'A METHOD FOR THE
C        DETERMINATION OF APPROXIMATE SYSTEM TRANSFER
C        FUNCTION', CHEMICAL ENGINEERING SCIENCE, VOL. 18,
C        PP.189-202, (1963).
C
C
C

      DIMENSION OMEGA(50),OMEG2(50),AMAG(50)
      DIMENSION FTER1(50),FPHI(50),FERR(50),FZ1(50)
      DIMENSION FERS2(100),FT12(100)
      DIMENSION STER1(50),STER2(50),SPHI(50),SERR(50)
     *,SZ1(50),
     1SZ2(50)
      DIMENSION SA(10,20),SC(10,10)
      DIMENSION SERS2(100),ST12(100),ST22(100)
      DIMENSION TTER1(50),TTER2(50),TTER3(50),TPHI(50)
     *,TERR(50),
     1 TZ1(50),TZ2(50),TZ3(50)
      DIMENSION TA(10,20),TC(10,10)
      DIMENSION TERS2(100),TT12(100),TT22(100),TT32(100)
```

SUBROUTINE BL123 ...(CONT'D)

```
C
C        FIT THE AMPLITUDE RATIO DATA BY FIRST ORDER
C        TRANSFER FUNCTION

      FT12(1) = 100.0
      IFP = 1
      WRITE (6,5206)
 5206 FORMAT (1H1)
 1000 CONTINUE
      WRITE (6,5205) IFP
 5205 FORMAT (///8X,'TRIAL NUMBER'I3//)

C        A MAXIMUM OF 20 INITIAL GUESSES IS PERMITTED

      IF(IFP-20) 5204,5204,1998
 1998 CONTINUE
      WRITE (6,5207)
 5207 FORMAT (///9X,'FAILED TO CONVERGE TO A PHYSICALLY
     * REALIZABLE SOLUT
     1ION AFTER 10 TRIALS')
      GO TO 1999
 5204 CONTINUE
      ITF = 1

C        START THE ITERATION PROCEDURE
C

      FERS2(ITF) = 0.0
      DO 1001  IW=1,NFQ
      OMEG2(IW) = OMEGA(IW)*OMEGA(IW)
      FTER1(IW) = FT12(ITF)*OMEG2(IW)+1.0
      FPHI(IW) = 1.0/SQRT(ABS(FTER1(IW)))
      FERR(IW) = AMAG(IW)-FPHI(IW)
      FERS2(ITF) = FERS2(ITF)+FERR(IW)*FERR(IW)
 1001 CONTINUE
      WRITE (6,148)
  148 FORMAT(10X,'ITERATION',7X,'(TAU1)**2',8X,'SUM OF
     * ERRORS'//)
 1002 CONTINUE
      WRITE (6,149) ITF,FT12(ITF),FERS2(ITF)
  149 FORMAT (1H0,12X,I3,5X,E15.6,4X,E15.6)
      ALPHA = 1.0
      BETA = 0.25
      FC1 =0.0
      FZ12 = 0.0

      DO 1003  IW=1,NFQ
      OMEG2(IW) = OMEGA(IW)*OMEGA(IW)
      FTER1(IW) = FT12(ITF)*OMEG2(IW)+1.0
```

SUBROUTINE BL123 ...(CONT'D)

```
      FPHI(IW) = 1.0/SQRT(ABS(FTER1(IW)))
      FERR(IW) = AMAG(IW)-FPHI(IW)
      FZ1(IW) = -0.50*OMEG2(IW)*FPHI(IW)**3
      FZ12 = FZ12+FZ1(IW)*FZ1(IW)
      FC1 = FC1+FERR(IW)*FZ1(IW)
 1003 CONTINUE
      DFT12 = FC1/FZ12
      FD1 = DFT12*FC1
      FDT = FD1
      IF(FDT) 1004,1005,1005
 1004 CONTINUE
      FDT = -FDT
      DFT12 = -DFT12
 1005 CONTINUE
      ITF1 = ITF+1
      FT12(ITF1) = FT12(ITF)+DFT12

C
C        IF (TAU1)**2 IS NEGATIVE, TRY ANOTHER GUESS

      IF(FT12(ITF1)) 5200,5200,5201
 5200 CONTINUE
      FT12(1) = ABS(FT12(ITF1))
      IFP = IFP+1
      GO TO 1000
 5201 CONTINUE

C        CHECH WHETHER THE METHOD CONVERGES OR NOT

      IF(ABS(DFT12)-  0.01) 1007,1007,1008
 1008 CONTINUE
      FERS2(ITF1) = 0.0
      DO 1006  IW=1,NFQ
      OMEG2(IW) = OMEGA(IW)*OMEGA(IW)
      FTER1(IW) = FT12(ITF1)*OMEG2(IW)+1.0
      FPHI(IW) = 1.0/SQRT(ABS(FTER1(IW)))
      FERR(IW) = AMAG(IW)-FPHI(IW)
      FERS2(ITF1) = FERS2(ITF1)+FERR(IW)*FERR(IW)
 1006 CONTINUE
      FISCE = BETA*FDT*(2.0*ALPHA-ALPHA*ALPHA)
      DELSF = FERS2(ITF)-FERS2(ITF1)
      IF(DELSF-FISCE+1.0E-06) 1009,1010,1010
 1009 CONTINUE
      ALPHA = ALPHA/2.0
      DFB12 = ALPHA*DFT12
      FT12(ITF1) = FT12(ITF)+DFB12
      GO TO 1008
 1010 CONTINUE
      FFFF = (FERS2(ITF)-FERS2(ITF1))/FERS2(ITF1)
      IF(ABS(FFFF)-0.001) 1007,1007,1443
```

SUBROUTINE BL123 ...(CONT'D)

```
 1443 CONTINUE
      ITF = ITF+1
      FT12(ITF) = FT12(ITF1)
      FERS2(ITF) = FERS2(ITF1)
C
C         A MAXIMUM OF 50 INITIAL ASSUMPTIONS IS PERMITTED
C         FOR EACH INITIAL ASSUMPTION
C
      IF(ITF1- 50) 1521,1521,1522
 1522 CONTINUE
      WRITE (6,1523)
 1523 FORMAT (1H0,12X,'THIS METHOD FAILED TO CONVERGE IN  50
     * ITERATIONS'
     1//)
      GO TO 1999
 1521 CONTINUE
      GO TO 1002
 1007 CONTINUE
      IF (FT12(ITF1)) 1700,1700,1701
 1701 CONTINUE
      FT1 = SQRT(FT12(ITF1))
C
C         WRITE OUT THE RESULTS
C
      WRITE(6,150)
  150 FORMAT(///'0',8X,'FIRST ORDER TRANSFER FUNCTION
     * REPRESENTATION'/)
      WRITE (6,151) FT1
  151 FORMAT('0',10X,'TAU1 =',F10.3)
      WRITE (6,152) FERS2(ITF)
  152 FORMAT(//'0',10X,'SUM OF SQUARRED ERRORS IN FREQUENCY
     * DOMAIN IS ='
     1,E12.4)
      WRITE (6,153) ITF
  153 FORMAT (1H0,10X,'NUMBER OF ITERATIONS REQUIRED' I5)
      GO TO 1999
 1700 CONTINUE
      FT12(ITF1) = -FT12(ITF1)
      WRITE (6,1705)
 1705 FORMAT (//1H0,8X,'THIS PROBLEM CONVERGES TO A SOLUTION
     * WHICH IS PH
     1YSICALLY UNREALIZABLE')
 1999 CONTINUE
C
C         FIT THE AMPLITUDE RATIO DATA BY TWO FIRST ORDER
C         TRANSFER FUNCTIONS IN CASCADE
C
      WRITE (6,6206)
 6206 FORMAT (1H1)
```

SUBROUTINE BL123 ...(CONT'D)

```
      ST12(1) = FT12(ITF1)
      ST22(1) = 0.50*ST12(1)
      ISP = 1
 2000 CONTINUE
      WRITE (6,6205) ISP
 6205 FORMAT (///8X,'TRIAL NUMBER',I3//)
C         A MAXIMUM OF 20 INITIAL GUESSES IS PERMITTED
      IF(ISP-20) 6204,6204,2998
 2998 CONTINUE
      WRITE (6,6207)
 6207 FORMAT (///9X,'FAILED TO CONVERGE TO A PHYSICALLY
     * REALIZABLE SOLUT
     1ION AFTER 20 TRIALS')
      GO TO 2999
 6204 CONTINUE
C         START THE ITERATION PROCEDURE
      ITS = 1
      SERS2(ITS) = 0.0
      DO 2001  IW=1,NFQ
      OMEG2(IW) = OMEGA(IW)*OMEGA(IW)
      STER1(IW) = ST12(ITS)*OMEG2(IW)+1.0
      STER2(IW) = ST22(ITS)*OMEG2(IW)+1.0
      SPHI(IW) = 1.0/SQRT(ABS(STER1(IW)*STER2(IW)))
      SERR(IW) = AMAG(IW)-SPHI(IW)
      SERS2(ITS) = SERS2(ITS)+SERR(IW)*SERR(IW)
 2001 CONTINUE
      WRITE (6,248)
  248 FORMAT(10X,'ITERATION',7X,'(TAU1)**2',9X,'(TAU2)**2'
     *,8X,
     1'SUM OF ERRORS'//)
 2002 CONTINUE
      WRITE (6,249) ITS,ST12(ITS),ST22(ITS),SERS2(ITS)
  249 FORMAT (1H0,12X,I3,5X,E15.6,4X,E15.6,4X,E15.6)
      ALPHA = 1.0
      BETA = 0.25
      SC1 = 0.0
      SC2 = 0.0
      SZ11 = 0.0
      SZ12 = 0.0
      SZ22 = 0.0

      DO 2003  IW=1,NFQ
      OMEG2(IW) = OMEGA(IW)*OMEGA(IW)
      STER1(IW) = ST12(ITS)*OMEG2(IW)+1.0
      STER2(IW) = ST22(ITS)*OMEG2(IW)+1.0
```

SUBROUTINE BL123 ...(CONT'D)

```
      SPHI(IW) = 1.0/SQRT(ABS(STER1(IW)*STER2(IW)))
      SERR(IW) = AMAG(IW)-SPHI(IW)
      SZ1(IW) = -0.50*OMEG2(IW)*STER2(IW)*SPHI(IW)**3
      SZ2(IW) = -0.50*OMEG2(IW)*STER1(IW)*SPHI(IW)**3
      SZ11 = SZ11+SZ1(IW)*SZ1(IW)
      SZ12 = SZ12+SZ1(IW)*SZ2(IW)
      SZ22 = SZ22+SZ2(IW)*SZ2(IW)
      SC1 = SC1+SERR(IW)*SZ1(IW)
      SC2 = SC2+SERR(IW)*SZ2(IW)
 2003 CONTINUE
      SZ21 = SZ12
      NDIMS = 2
      SA(1,1) = SZ11
      SA(1,2) = SZ12
      SA(2,1) = SZ21
      SA(2,2) = SZ22
      SC(1,1) = SC1
      SC(2,1) = SC2
C
C        CALL SUBROUTINE SOLEQ TO SOLVE THE SYSTEM OF 2
C        EQUATIONS
C
      CALL SOLEQ(SA,SC,NDIMS,1,DET,-1)
      SDB1 = SC(1,1)
      SDB2 = SC(2,1)
      SD1 = SDB1*SC1
      SD2 = SDB2*SC2
      SDT = SD1+SD2
      IF(SDT) 2004,2005,2005
 2004 CONTINUE
      SDT = -SDT
      SDB1 = -SDB1
      SDB2 = -SDB2
 2005 CONTINUE
      ITS1 = ITS+1
      ST12(ITS1) = ST12(ITS)+SDB1
      ST22(ITS1) = ST22(ITS)+SDB2
C
C        CHECK WHETHER THE METHOD CONVERGES OR NOT
C
      IF(ABS(SDB1)-0.01)   2006,2006,2007
 2006 CONTINUE
      IF(ABS(SDB2)-0.01)   2008,2008,2007
 2007 CONTINUE
      SERS2(ITS1) = 0.0
      DO 2009  IW=1,NFQ
      OMEG2(IW) = OMEGA(IW)*OMEGA(IW)
      STER1(IW) = ST12(ITS1)*OMEG2(IW)+1.0
      STER2(IW) = ST22(ITS1)*OMEG2(IW)+1.0
      SPHI(IW) = 1.0/SQRT(ABS(STER1(IW)*STER2(IW)))
```

SUBROUTINE BL123 ...(CONT'D)

```
      SERR(IW) = AMAG(IW)-SPHI(IW)
      SERS2(ITS1) = SERS2(ITS1)+SERR(IW)*SERR(IW)
 2009 CONTINUE
      SISCE = BETA*SDT*(2.0*ALPHA-ALPHA*ALPHA)
      DELSS = SERS2(ITS)-SERS2(ITS1)
      IF(DELSS-SISCE+1.0E-06) 2010,2011,2011
 2010 CONTINUE
      ALPHA = ALPHA/2.0
      SDF1 = ALPHA*SDB1
      SDF2 = ALPHA*SDB2
      ST12(ITS1) = ST12(ITS)+SDF1
      ST22(ITS1) = ST22(ITS)+SDF2
      GO TO 2007
 2011 CONTINUE
      SSSS = (SERS2(ITS)-SERS2(ITS1))/SERS2(ITS1)
      IF(ABS(SSSS)-1.0E-3) 2008,2008,2037
 2037 CONTINUE
      ITS = ITS+1
      ST12(ITS) = ST12(ITS1)
      ST22(ITS) = ST22(ITS1)
      SERS2(ITS) = SERS2(ITS1)
C
C        A MAXIMUM OF 50 ITERATIONS IS PERMITTED FOR EACH
C        INITIAL ASSUMPTION

      IF(ITS1- 50) 2521,2521,2522
 2522 CONTINUE
      WRITE (6,2523)
 2523 FORMAT (1H0,12X,'THIS METHOD FAILED TO CONVERGE IN 100
     * ITERATIONS'
     1//)
      GO TO 2999
 2521 CONTINUE
      GO TO 2002
 2008 CONTINUE
      IF(ST12(ITS1)) 6200,6200,6201
 6200 CONTINUE
      ST12(1) = ABS(ST12(ITS1))
      ST12(1) = ABS(ST12(ITS1))
      ISP = ISP+1
      WRITE (6,2708)
      GO TO 2000
 6201 CONTINUE

C        IF (TAU1)**2 OR (TAU2)**2 IS NEGATIVE, TRY ANOTHER
C        GUESS

      IF(ST22(ITS1)) 6202,6202,6203
 6202 CONTINUE
```

SUBROUTINE BL123 ...(CONT'D)

```
      ST22(1) = ABS(ST22(ITS1))
      ST22(1) = ABS(ST22(ITS1))
      ISP = ISP+1
      WRITE (6,2708)
      GO TO 2000
 2708 FORMAT (//1H0,8X,'INITIAL ASSUMPTIONS OF TAU1 AND TAU2
     * ARE POOR ,
     1PHYSICALLY UNREALIZABLE')
 6203 CONTINUE
      ST1 = SQRT(ST12(ITS1))
      ST2 = SQRT(ST22(ITS1))
C
C         WRITE OUT THE RESULTS
C
      WRITE (6,250)
  250 FORMAT(///'0',8X,'SECOND ORDER TRANSFER FUNCTION
     * REPRESENTATION'/)
      WRITE (6,251) ST1,ST2
  251 FORMAT(/'0',10X,'TAU1 =',F10.3,10X,'TAU2 =',F10.3)
      WRITE (6,252) SERS2(ITS)
  252 FORMAT(//'0',10X,'SUM OF SQUARRED ERRORS IN FREQUENCY
     * DOMAIN IS ='
     1,E12.4)
      WRITE (6,253) ITS
  253 FORMAT (1H0,10X,'NUMBER OF ITERATIONS REQUIRED' I5)
 2999 CONTINUE
C
C
C         FIT THE AMPLITUDE RATIO DATA BY THREE FIRST ORDER
C         TRANSFER FUNCTIONS IN CASCADE
C
      WRITE (6,7206)
 7206 FORMAT (1H1)
      TT12(1) = FT12(ITF1)*0.80
      TT22(1) = FT12(ITF1)*0.50
      TT32(1) = FT12(ITF1)*0.30
      ITP = 1
 3000 CONTINUE
      WRITE (6,7205) ITP
 7205 FORMAT (///8X,'TRIAL NUMBER',I3//)
      IF (ITP-20) 7204,7204,3998
 3998 CONTINUE
      WRITE (6,7207)
 7207 FORMAT (///9X,'FAILED TO CONVERGE TO A PHYSICALLY
     * REALIZABLE SOLUT
     1ION AFTER 20 TRIALS')
      GO TO 3999
 7204 CONTINUE
C
C         START THE ITERATION PROCEDURE
```

SUBROUTINE BL123 ...(CONT'D)

```
      ITT = 1
      TERS2(ITT) = 0.0
      DO 3001  IW=1,NFQ
      OMEG2(IW) = OMEGA(IW)*OMEGA(IW)
      TTER1(IW) = TT12(ITT)*OMEG2(IW)+1.0
      TTER2(IW) = TT22(ITT)*OMEG2(IW)+1.0
      TTER3(IW) = TT32(ITT)*OMEG2(IW)+1.0
      TPHI(IW) = 1.0/SQRT(ABS(TTER1(IW)*TTER2(IW)
     **TTER3(IW)))
      TERR(IW) = AMAG(IW)-TPHI(IW)
      TERS2(ITT) =TERS2(ITT)+TERR(IW)*TERR(IW)
3001  CONTINUE
      WRITE (6,348)
 348  FORMAT (10X,'ITERATION',7X,'(TAU1)**2',9X,'(TAU2)**2'
     *,9X,'(TAU3)**
     12',8X,'SUM OF ERRORS'//)
3002  CONTINUE
      WRITE (6,349) ITT,TT12(ITT),TT22(ITT),TT32(ITT)
     *,TERS2(ITT)
 349  FORMAT (1H0,12X,I3,5X,E15.6,4X,E15.6,4X,E15.6,4X
     *,E15.6)


      ALPHA = 1.0
      BETA = 0.25
      TC1 = 0.0
      TC2 = 0.0
      TC3 = 0.0
      TZ11 = 0.0
      TZ12 = 0.0
      TZ13 = 0.0
      TZ22 = 0.0
      TZ23 = 0.0
      TZ33 = 0.0
      DO 3003  IW=1,NFQ
      OMEG2(IW) = OMEGA(IW)*OMEGA(IW)
      TTER1(IW) = TT12(ITT)*OMEG2(IW)+1.0
      TTER2(IW) = TT22(ITT)*OMEG2(IW)+1.0
      TTER3(IW) = TT32(ITT)*OMEG2(IW)+1.0
      TPHI(IW) = 1.0/SQRT(ABS(TTER1(IW)*TTER2(IW)
     **TTER3(IW)))
      TERR(IW) = AMAG(IW)-TPHI(IW)
      TZ1(IW) = -0.50*OMEG2(IW)*TTER2(IW)*TTER3(IW)*TPHI(IW)
     ***3
      TZ2(IW) = -0.50*OMEG2(IW)*TTER1(IW)*TTER3(IW)*TPHI(IW)
     ***3
      TZ3(IW) = -0.50*OMEG2(IW)*TTER1(IW)*TTER2(IW)*TPHI(IW)
     ***3
```

SUBROUTINE BL123 ...(CONT'D)

```
      TZ11 = TZ11+TZ1(IW)*TZ1(IW)
      TZ12 = TZ12+TZ1(IW)*TZ2(IW)
      TZ13 = TZ13+TZ1(IW)*TZ3(IW)
      TZ22 = TZ22+TZ2(IW)*TZ2(IW)
      TZ23 = TZ23+TZ2(IW)*TZ3(IW)
      TZ33 = TZ33+TZ3(IW)*TZ3(IW)
      TC1 = TC1+TERR(IW)*TZ1(IW)
      TC2 = TC2+TERR(IW)*TZ2(IW)
      TC3 = TC3+TERR(IW)*TZ3(IW)
 3003 CONTINUE
      TZ21 = TZ12
      TZ31 = TZ13
      TZ32 = TZ23
      TA(1,1) = TZ11
      TA(1,2) = TZ12
      TA(1,3) = TZ13
      TA(2,1) = TZ21
      TA(2,2) = TZ22
      TA(2,3) = TZ23
      TA(3,1) = TZ31
      TA(3,2) = TZ32
      TA(3,3) = TZ33
      NDIMT = 3
      TC(1,1) = TC1
      TC(2,1) = TC2
      TC(3,1) = TC3

C        CALL SUBROUTINE SOLEQ TO SOLVE A SYSTEM OF 3
C        EQUATIONS

      CALL SOLEQ(TA,TC,NDIMT,1,DET,-1)
      TDB1 = TC(1,1)
      TDB2 = TC(2,1)
      TDB3 = TC(3,1)
      TD1 = TDB1*TC1
      TD2 = TDB2*TC2
      TD3 = TDB3*TC3
      TDT = TD1+TD2+TD3
      IF(TDT) 3004,3005,3005
 3004 CONTINUE
      TDB1 = -TDB1
      TDB2 = -TDB2
      TDB3 = -TDB3
      TDT = -TDT
 3005 CONTINUE
      ITT1 = ITT+1
      TT12(ITT1) = TT12(ITT)+TDB1
      TT22(ITT1) = TT22(ITT)+TDB2
      TT32(ITT1) = TT32(ITT)+TDB3
```

SUBROUTINE BL123 ...(CONT'D)

```
C        CHECK WHETHER THE METHOD CONVERGES OR NOT
      IF(ABS(TDB1)-0.10) 3006,3006,3007
 3006 CONTINUE
      IF(ABS(TDB2)-0.10) 3008,3008,3007
 3008 CONTINUE
      IF(ABS(TDB3)-0.10) 3020,3020,3007
 3007 CONTINUE
      TDF1 = TDB1
      TDF2 = TDB2
      TDF3 = TDB3
 3888 CONTINUE
      TERS2(ITT1) = 0.0
      DO 3009  IW=1,NFQ
      OMEG2(IW) = OMEGA(IW)*OMEGA(IW)
      TTER1(IW) = TT12(ITT)*OMEG2(IW)+1.0
      TTER2(IW) = TT22(ITT)*OMEG2(IW)+1.0
      TTER3(IW) = TT32(ITT)*OMEG2(IW)+1.0
      TPHI(IW) = 1.0/SQRT(ABS(TTER1(IW)*TTER2(IW)
     **TTER3(IW)))
      TERR(IW) = AMAG(IW)-TPHI(IW)
      TERS2(ITT) =TERS2(ITT)+TERR(IW)*TERR(IW)
      TERS2(ITT) =TERS2(ITT)+TERR(IW)*TERR(IW)
      TERS2(ITT1) = TERS2(ITT1)+TERR(IW)*TERR(IW)
 3009 CONTINUE
      TISCE = BETA*TDT*(2.0*ALPHA-ALPHA*ALPHA)
      DELST = TERS2(ITT)-TERS2(ITT1)
      IF(DELST-TISCE) 3010,3011,3011
 3010 CONTINUE
      ALPHA = ALPHA/2.0
      TDB1 = ALPHA*TDF1
      TDB2 = ALPHA*TDF2
      TDB3 = ALPHA*TDF3
      TT12(ITT1) = TT12(ITT)+TDB1
      TT22(ITT1) = TT22(ITT)+TDB2
      TT32(ITT1) = TT32(ITT)+TDB3
      GO TO 3888
 3011 CONTINUE
      TTTT = (TERS2(ITT)-TERS2(ITT1))/TERS2(ITT1)
      IF(ABS(TTTT)-1.0E-3) 3020,3020,3579
 3579 CONTINUE
      ITT = ITT+1
      TT12(ITT) = TT12(ITT1)
      TT22(ITT) = TT22(ITT1)
      TT32(ITT) = TT32(ITT1)
      TERS2(ITT) = TERS2(ITT1)
C
C        A MAXIMUM OF 50 ITERATIONS IS PERMITTED FOR EACH
C        INITIAL ASSUMPTION
C
```

SUBROUTINE BL123 ...(CONT'D)

```
      IF(ITT1- 50) 7521,7521,7522
 7522 CONTINUE
      WRITE (6,7523)
 7523 FORMAT (1H0,12X,'THIS METHOD FAILED TO CONVERGE IN  50
     * ITERATIONS'
     1//)
      GO TO 3999
 7521 CONTINUE
      GO TO 3002
 3020 CONTINUE

C         IF (TAU1)**2, (TAU2)**2 OR (TAU3)**2 IS NEGATIVE,
C         TRY ANOTHER GUESS

      IF(TT12(ITT1)) 7200,7200,7201
 7200 CONTINUE
      TT12(1) = ABS(TT12(ITT1))
      TT22(1) = ABS(TT22(ITT1))
      TT32(1) = ABS(TT32(ITT1))
      WRITE (6,3710)
      ITP = ITP+1
      GO TO 3000
 7201 CONTINUE
      IF(TT22(ITT1)) 7301,7301,7302
 7301 CONTINUE
      TT12(1) = ABS(TT12(ITT1))
      TT22(1) = ABS(TT22(ITT1))
      TT32(1) = ABS(TT32(ITT1))
      ITP = ITP+1
      WRITE (6,3710)
      GO TO 3000
 7302 CONTINUE
      IF(TT32(ITT1)) 7303,7303,7304
 7303 CONTINUE
      TT12(1) = ABS(TT12(ITT1))
      TT22(1) = ABS(TT22(ITT1))
      TT32(1) = ABS(TT32(ITT1))
      ITP = ITP+1
      WRITE (6,3710)
      GO TO 3000
 3710 FORMAT (//1H0,8X,'INITIAL ASSUMPTIONS OF TAU1 , TAU2 ,
     * TAU3 ARE PO
     1OR')
 7304 CONTINUE

C          WRITE OUT THE RESULTS

      TT1 = SQRT(TT12(ITT1))
      TT2 = SQRT(TT22(ITT1))
      TT3 = SQRT(TT32(ITT1))
```

SUBROUTINE BL123 ...(CONT'D)

```
      WRITE (6,350)
  350 FORMAT(///'0',8X,'THIRD ORDER TRANSFER FUNCTION
     * REPRESENTATION'/)
      WRITE (6,351) TT1,TT2,TT3
  351 FORMAT(/'0',10X,'TAU1 =', F7.3, 6X,'TAU2 =', F7.3, 6X
     *,'TAU3 =', F7
     1.3)
      WRITE (6,352) TERS2(ITT1)
  352 FORMAT(//'0',10X,'SUM OF SQUARRED ERRORS IN FREQUENCY
     * DOMAIN IS ='
     1,E12.4)
 3999 CONTINUE
      RETURN
      END
```

SUBROUTINE BLUND

```
      SUBROUTINE BLUND (OMEGA,AMAG,NFQ)
C
C
C                   SUBROUTINE  BLUND
C                   -----------------
C
C
C     PURPOSE
C        FIT THE AMPLITUDE RATIO DATA BY UNDERDAMPED SECOND
C        ORDER TRANSFER FUNCTIONS
C
C     DESCRIPTION OF PARAMETERS
C        OMEGA     FREQUENCY
C        AMAG      MAGNITUDE RATIO
C        NFQ       NUMBER OF DATA POINTS
C
C     USAGE
C        CALL BLUND (OMEGA,AMAG,NFQ)
C
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C        SOLEQ
C
C     METHOD
C        BAILEY AND LAW'S NON LINEAR REGRESSION TECHNIQUE
C
C     REFERENCE
C        BAILEY, R.V., AND LAW, V.J., 'A METHOD FOR THE
C        DETERMINATION OF APPROXIMATE SYSTEM TRANSFER
C        FUNCTION', CHEMICAL ENGINEERING SCIENCE, VOL. 18,
C        PP.189-202, (1963).
C
C

      DIMENSION OMEGA(50),OMEG2(50),AMAG(50)
      DIMENSION UTER1(50),UTER2(50),UPHI(50),UERR(50)
     *,UZ1(50),UZ2(50)
      DIMENSION UA(10,20),UC(10,10)
      DIMENSION UERS2(100),UTT1(100),UTT2(100)
      WRITE (6,400)
  400 FORMAT (1H1)
      UTT1(1) = 120.0
      UTT2(1) = 11.0
      IUP = 1
 4000 CONTINUE
      WRITE (6,402) IUP
  402 FORMAT (///8X,'TRIAL NUMBER',I3//)
C
C        A MAXIMUM OF 20 INITIAL GUESSES IS PERMITTED
```

SUBROUTINE BLUND ...(CONT'D)

```
      IF(IUP-20) 4004,4004,4002
 4002 CONTINUE
      WRITE (6,404)
  404 FORMAT (///9X,'FAILED TO CONVERGE AFTER 20 TRIALS')
      GO TO 4999
 4004 CONTINUE
C
C         START THE ITERATION PROCEDURE
C
      ITU = 1
      UERS2(ITU) = 0.0
      DO 4006  IW=1,NFQ
      UTER1(IW) = 1.0-UTT1(ITU)*OMEGA(IW)*OMEGA(IW)
      UTER2(ITU) = UTT2(ITU)*OMEGA(IW)
      UPHI(IW) = 1.0/SQRT(UTER1(ITU)*UTER1(ITU)+UTER2(ITU)
     **UTER2(ITU))
      UERR(IW) = AMAG(IW)-UPHI(IW)
      UERS2(ITU) = UERS2(ITU)+UERR(IW)*UERR(IW)
 4006 CONTINUE
      WRITE (6,406)
  406 FORMAT (10X,'ITERATION',11X,'A',13X,'B',11X,'SUM OF
     * ERRORS'//)
 4009 CONTINUE
      WRITE (6,456) ITU,UTT1(ITU),UTT2(ITU),UERS2(ITU)
  456 FORMAT (1H0,12X,I3,5X,E15.6,4X,E15.6,4X,E15.6)


      ALPHA = 1.0
      BETA = 0.25
      UC1 = 0.0
      UC2 = 0.0
      UZ11 = 0.0
      UZ12 = 0.0
      UZ22 = 0.0
      DO 4008  IW=1,NFQ
      UTER1(IW) = 1.0-UTT1(ITU)*OMEGA(IW)*OMEGA(IW)
      UTER2(IW) = UTT2(ITU)*OMEGA(IW)
      UPHI(IW) = 1.0/SQRT(UTER1(IW)*UTER1(IW)+UTER2(IW)
     **UTER2(IW))
      UERR(IW) = AMAG(IW)-UPHI(IW)
      UZ1(IW) = -OMEGA(IW)*OMEGA(IW)*UPHI(IW)**3*(UTT1(ITU)
     **OMEGA(IW)*
     1OMEGA(IW)-1.0)
      UZ2(IW) = -OMEGA(IW)*OMEGA(IW)*UPHI(IW)**3*UTT2(ITU)
      UZ11 = UZ11+UZ1(IW)*UZ1(IW)
      UZ12 = UZ12+UZ1(IW)*UZ2(IW)
      UZ22 = UZ22+UZ2(IW)*UZ2(IW)
      UC1 = UC1+UERR(IW)*UZ1(IW)
      UC2 = UC2+UERR(IW)*UZ2(IW)
 4008 CONTINUE
```

SUBROUTINE BLUND ...(CONT'D)

```
      UZ21 = UZ12
      NDIMU = 2
C        SOLE A SYSTEM OF 2 EQUATIONS
      UA(1,1) = UZ11
      UA(1,2) = UZ12
      UA(2,1) = UZ21
      UA(2,2) = UZ22
      UC(1,1) = UC1
      UC(2,1) = UC2
      CALL SOLEQ(UA,UC,NDIMU,1,DET,-1)
      UDB1 = UC(1,1)
      UDB2 = UC(2,1)
      UD1 = UDB1*UC1
      UD2 = UDB2*UC2
      UDT = UD1+UD2
      IF(UDT) 4600,4600,4601
 4600 CONTINUE
      UDT = -UDT
      UDB1 = -UDB1
      UDB2 = -UDB2
 4601 CONTINUE
      ITU1 = ITU+1
      UTT1(ITU1) = UTT1(ITU)+UDB1
      UTT2(ITU1) = UTT2(ITU)+UDB2
C        CHECK WHETHER THE METHOD CONVERGES OR NOT
      IF(ABS(UDB1)-0.010)  4608,4608,4100
 4608 CONTINUE
      IF(ABS(UDB2)-0.010) 4500,4500,4100
 4100 CONTINUE
      UERS2(ITU1) = 0.0
      DO 4102  IW=1,NFQ
      OMEG2(IW) = OMEGA(IW)*OMEGA(IW)
      UTER1(IW) = 1.0-UTT1(ITU1)*OMEG2(IW)
      UTER2(IW) = UTT2(ITU1)*OMEGA(IW)
      UPHI(IW) = 1.0/SQRT(UTER1(IW)*UTER1(IW)+UTER2(IW)
     **UTER2(IW))
      UERR(IW) = AMAG(IW)-UPHI(IW)
      UERS2(ITU1) = UERS2(ITU1)+UERR(IW)*UERR(IW)
 4102 CONTINUE
      UISCE = BETA*UDT*(2.0*ALPHA-ALPHA*ALPHA)
      DELSU = UERS2(ITU)-UERS2(ITU1)
      IF(DELSU-UISCE+1.0E-06) 4104,4104,4106
 4104 CONTINUE
      ALPHA = ALPHA/2.0
      UDF1 = ALPHA*UDB1
      UDF2 = ALPHA*UDB2
```

SUBROUTINE BLUND ...(CONT'D)

```
      UTT1(ITU1)= UTT1(ITU)+UDF1
      UTT2(ITU1) = UTT2(ITU)+UDF2
      GO TO 4100
 4106 CONTINUE
      ITU = ITU+1
      UTT1(ITU) = UTT1(ITU1)
      UTT2(ITU) = UTT2(ITU1)
      UERS2(ITU) = UERS2(ITU1)
      IF(ITU-50) 4108,4108,4110

C         FAILED TO CONVERGE

 4110 CONTINUE
      WRITE (6,410)
  410 FORMAT (1H0,12X,'THIS METHOD FAILED TO CONVERGE IN 50
     * ITERATIONS')
      GO TO 4999
 4108 CONTINUE
      GO TO 4009
 4500 CONTINUE
      IF(UTT1(ITU1)) 4200,4200,4202
 4200 CONTINUE
      UTT1(1) = ABS(UTT1(ITU1))
      UTT2(1) = ABS(UTT2(ITU1))
      IUP = IUP+1
      WRITE (6,412)
 4202 CONTINUE
      IF(UTT2(ITU1)) 4204,4204,4206
 4204 CONTINUE
      UTT1(1) = ABS(UTT1(ITU1))
      UTT2(1) = ABS(UTT2(ITU1))
      IUP = IUP+1
      WRITE (6,412)
      GO TO 4000
  412 FORMAT (//1H0,8X,'INITIAL ASSUMPTIONS ARE POOR,START
     * ANOTHER GUESS
     1')
 4206 CONTINUE

C         WRITE OUT THE RESULTS

      A = UTT1(ITU)
      B = UTT2(ITU)
      WRITE (6,450)
  450 FORMAT (////'SECOND ORDER TRANSFER FUNCTION
     * REPRESENTATION'/)
      WRITE (6,451) A,B
  451 FORMAT (//10X,'A =' ,F10.3,10X,'B =',F10.3)
      WRITE (6,453) UERS2(ITU)
  453 FORMAT (///10X,'SUM OF SQUARES ERRORS IN FREQUENCY
```

SUBROUTINE BLUND ...(CONT'D)

```
    * DOMAIN IS ='
    1,E12.4)
     WRITE (6,454) ITU
 454 FORMAT(1H0,10X,'NUMBER OF ITERATIONS REQUIRED',I5)
4999 CONTINUE
     RETURN
     END
```

SUBROUTINE SOLEQ

```
      SUBROUTINE SOLEQ(A,B,N,NSYS,DET,FLAG)
C
C
C                    SUBROUTINE  SOLEQ
C                    -----------------
C
C
C     PURPOSE
C        CALCULATE THE DETERMINANT OF MATRIX A, THE INVERSE
C        OF MATRIX A, OR SOLVE THE SYSTEMS OF EQUATIONS
C        A*X = B
C
C     DESCRIPTION OF PARAMETERS
C        A          LOCATION OF AUGMENTED MATRIX A
C        B          LOCATION OF MATRIX B
C        N          ORDER OF MATRIX A
C        NSYS       NUMBER OF COLUMNS IN MATRIX B
C        DET        DETERMINANT OF MATRIX A
C        FLAG       PROGRAM CONTROL FLAG
C                    0 ... CALCULATE THE DETERMINANT ONLY
C                    1 ... CALCULATE THE INVERSE MATRIX AND
C                   THE DETERMINANT
C                   -1 ... SOLVE THE SYSTEMS OF EQUATIONS
C
C     USAGE
C        CALL SOLEQ (A, B, N, NSYS, DET, FLAG)
C
C     METHOD
C        GAUSSIAN ELIMINATION WITH PIVOTING
C
C     REFERENCE
C        CONTE, S.D., 'ELEMENTARY NUMERICAL ANALYSIS', PP.
C        156-176, MC GRAW HILL CO., NEW YORK, (1965).
C
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C        NONE
C
C
      INTEGER FLAG
      DIMENSION A(10,20),B(10,10),X(20)
      SIGN = 1
      MARK = 0
      NM1 = N-1
      NP1 = N+1
      NN = 2.0*N
      NPLSY = N+NSYS
      IF(FLAG) 1020,1020,1010
 1010 CONTINUE
```

SUBROUTINE SOLEQ ...(CONT'D)

```
      DO 1012  K=1,N
      DO 1012  J=1,N
      B(K,J) = 0.0
 1012 CONTINUE
      DO 1014 J=1,N
      B(J,J) = 1.0
 1014 CONTINUE
      NPLSY = NN
 1020 CONTINUE
C        CONSTRUCTION OF THE AUGMENTED MATRIX
      DO 1000  I=1,N
      DO 1000  J=NP1,NPLSY
      K = J-N
      A(I,J) = B(I,K)
 1000 CONTINUE

      DO 1190  I=1,NM1
C        PICK UP PIVOT ELEMENT
      MAX = I
      AMAX = ABS(A(I,I))
      IP1 = I+1
      DO 1040  K=IP1,N
      IF(ABS(A(K,I))-AMAX) 1040,1040,1030
 1030 CONTINUE
      MAX = K
      AMAX = ABS(A(K,I))
 1040 CONTINUE
      IF(MAX-I) 1050,1080,1050
 1050 CONTINUE
C        ROW INTERCHANGES
      DO 1060  L=I,NPLSY
      TEMP = A(I,L)
      A(I,L) = A(MAX,L)
      A(MAX,L) = TEMP
 1060 CONTINUE
      SIGN = -SIGN
 1080 CONTINUE
      DO 1180  J=IP1,N
      IF(ABS(A(J,I))-1.0E-10) 1120,1120,1110
 1110 CONTINUE
      CONST = -A(J,I)/A(I,I)
      DO 1120  L=I,NPLSY
      A(J,L) = A(J,L)+A(I,L)*CONST
```

SUBROUTINE SOLEQ ...(CONT'D)

```
 1120 CONTINUE
 1180 CONTINUE
 1190 CONTINUE

      TEMP = 1.0

C     COMPUTE DETERMINANT OF MATRIX  A

      DO 2030  I=1,N
      IF(ABS(A(I,I))-1.0E-10) 2010,2010,2020
 2010 CONTINUE

C        CONTENT OF MARK IS SET EQUAL TO 1 - MATRIX A IS
C        SINGULAR

      MARK = 1
      WRITE (6,100)
  100 FORMAT (///10X,'MATRIX A IS SINGULAR - EXIT')
      GO TO 2040
 2020 CONTINUE
      TEMP = TEMP*A(I,I)
 2030 CONTINUE
      DET = SIGN*TEMP
 2040 CONTINUE
      IF(FLAG) 3000,9999,3000
 3000 CONTINUE
      IF(FLAG-1) 3020,3010,3020
 3010 CONTINUE
      IF(MARK-1) 3020,9999,3020
 3020 CONTINUE

C        BACK SUBSTITUTE

      DO 4050  I=NP1,NPLSY
      K = N
 4000 CONTINUE
      X(K) = A(K,I)
      IF(K-N) 4010,4020,4010
 4010 CONTINUE
      JP1 = K+1
      DO 4020  J=JP1,N
      X(K) = X(K)-A(K,J)*X(J)
 4020 CONTINUE
      X(K) = X(K)/A(K,K)
      IF(K-1) 4030,4040,4030
 4030 CONTINUE
      K = K-1
      GO TO 4000
 4040 CONTINUE
```

SUBROUTINE SOLEQ ...(CONT'D)

```
      DO 4050  L=1,N
      A(L,I) = X(L)
 4050 CONTINUE
C
C        THE INVERSE OR THE SOLUTION MATRIX X WILL BE STORED
C        IN THE MATRIX B
C
      DO 5000  I=1,N
      DO 5000  J=NP1,NPLSY
      K = J-N
      B(I,K) = A(I,J)
 5000 CONTINUE
 9999 RETURN
      END
```

MAINLINE FDCPO

```
      MAINLINE FDCPO
C
C
C            ***************************
C            *                         *
C            *    MAINLINE  FDCPO      *
C            *    ---------------      *
C            *                         *
C            ***************************
C
C
C     PURPOSE
C        DETERMINE THE VALUES OF FOURIER COEFFICIENTS WHICH
C        CAN BE USED TO APPROXIMATE THE TRANSFER FUNCTION
C        OF A LINEAR SYSTEM FROM ITS FREQUENCY RESPONSE
C
C     DESCRIPTION OF PARAMETERS
C        OMEGA    FREQUENCY
C        AMAG     MAGNITUDE OF THE BODE PLOT
C        NFQ      NUMBER OF INPUT DATA POINTS
C        INDEX    PROGRAM CONTROL FLAG
C                  1 ... PHASE LAGS ARE GIVEN IN DEGREES
C                 -1 ... PHASE LAGS ARE GIVEN IN RADIANS
C
C     USAGE
C        ENTER DATA AS REQUIRED
C
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C        LEASQ, QSF
C
C     METHOD
C        CHEN AND PHILIP'S METHOD
C
C     REFERENCE
C        CHEN, C.F., AND PHILIP, B.L., 'GRAPHICAL DETERMINA-
C        TION OF TRANSFER FUNCTION COEFFICIENTS FROM ITS
C        FREQUENCY RESPONSE', A.I.E.E. TRANS., APPLICATIONS
C        AND INDUSTRY, PP. 42-45, MARCH, 1963.
C
C     REMARKS
C        THIS METHOD IS RESTRICTED TO MINIMUM PHASE TRANSFER
C        FUNCTIONS
C
C

      DIMENSION AREAL(120), AMAT(120), AFOR(120), PHICN(50)
      DIMENSION OMEGA(50),AMAG(50),PHASE(50)
      DIMENSION PMAG(120),PHI(120),ACOEF(11),AF(120)
     *,AFOUR(25),
```

MAINLINE FDCPO ...(CONT'D)

```
     1EXPRS(120)
      PI = 3.141596
      DELPH = 0.02*PI
      READ (5,20) NCASE
   20 FORMAT (I5)
      DO 9999 KJ=1,NCASE
      READ (5,1) NFQ,INDEX
    1 FORMAT (2I5)
      READ (5,333) (OMEGA(I),AMAT(I),PHASE(I),I=1,NFQ)
  333 FORMAT(10X,F9.4,17X,F8.3,6X,F8.3)
C
C        IF INDEX = 1 CONVERT THE PHASE LAGS FROM DEGREES TO
C        RADIANS
C
      IF(INDEX-1) 2460,2470,2460
 2470 CONTINUE
      DO 2480  I=1,NFQ
      PHASE(I) = PHASE(I)*PI/180.0
 2480 CONTINUE
 2460 CONTINUE
C
C        COMPUTE REAL PARTS OF THE TRANSFER FUNCTION
C
      DO 2500  I=1,NFQ
      AMAG(I) = AMAT(I)/AMAT(1)
      AREAL(I) = AMAG(I)*COS(PHASE(I))
 2500 CONTINUE
C
C        CHANGE THE INDEPENDENT VARIABLE FROM OMEGA TO PHICN
C
      DO 1000  IW=1,NFQ
      PHICN(IW) = 2.0*ATAN(OMEGA(IW))
 1000 CONTINUE
      WRITE (6,521)  (OMEGA(IW),AREAL(IW),PHICN(IW),IW=1
     *,NFQ)
  521 FORMAT (1H0,3E15.6)
      NPOWR = 8
C
C        CALCULATE THE REAL PARTS OF THE MAGNITUDE RATIOS
C        FROM PHI = 0.0 TO PHI = 2.0*PI
C
      CALL LEASQ(AREAL,PHICN,NFQ,NPOWR,ACOEF)
      PHI(1) = 0.0
      DO  1002  IPC=1,51
      PMAG(IPC) = ACOEF(1)
      DO 1004  K=1,NPOWR
      PMAG(IPC) = PMAG(IPC)+ACOEF(K+1)*PHI(IPC)**K
 1004 CONTINUE
      PHI(IPC+1) = PHI(IPC)+DELPH
 1002 CONTINUE
```

```
      DO 1200  JINV=52,101
      JDUM = 102-JINV
      PMAG(JINV) = PMAG(JDUM)
      PHI(JINV) = PHI(JINV-1)+DELPH
 1200 CONTINUE
      WRITE (6,10)
   10 FORMAT (///10X,'VALUES OF FOURIER COEFFICIENTS'/)
C
C         EVALUATE ALL FOURIER COEFFICIENTS BY SIMPSON'S
C         METHOD
C
      CALL QSF(DELPH,PMAG,AFOR,101)
      AOFOU = AFOR(101)/(2.0*PI)
      WRITE (6,9) AOFOU
    9 FORMAT (1HO,12X,'A ( 0)  =',E14.6)
      DO 1010  N=1,20
      DO 1012  IPC=1,101
      EXPRS(IPC) = PMAG(IPC)*COS(N*PHI(IPC))
 1012 CONTINUE
      CALL QSF(DELPH,EXPRS,AF,101)
      AFOUR(N) = AF(101)/PI
C
C         WRITE OUT FOURIER COEFFICIENTS
C
      WRITE (6,11) N,AFOUR(N)
   11 FORMAT(1HO,12X,'A (',I2,')  =',E14.6)
 1010 CONTINUE
 9999 CONTINUE
      CALL EXIT
      END
```

SUBROUTINE LEASQ

```
      SUBROUTINE LEASQ (Y,X,N,M,A)
C
C
C                    SUBROUTINE  LEASQ
C                    -----------------
C
C
C     PURPOSE
C        THIS SUBROUTINE IS USED TO FIT ANY FUNCTION BY A
C        POLYNOMIAL USING LEAST SQUARE METHOD
C        THE POLYNOMIAL IS THAT OF THE FOLLOWING FORM
C        Y = A(M)*X**M+A(M-1)*X**(M-1)+ ... +A(1)*X+A(0)
C
C     DESCRIPTION OF PARAMETERS
C        Y          INPUT VECTOR, DEPENDENT VARIABLE
C        X          INPUT VECTOR, INDEPENDENT VARIABLE
C        N          DIMENSION OF INPUT VECTOR
C        M          DEGREE OF THE POLYNOMIAL
C        A          COEFFICIENTS OF THE POLYNOMIAL (M+1) COEF.
C
C     USAGE
C        CALL LEASQ (Y,X,N,M,A)
C
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C        NONE
C
C

      REAL X(50),Y(50),W(21),Z(11),A(11),B(11,12)
      LW = 2*M+1
      LB = M+2
      LZ = M+1
      DO 5  J=2,LW
    5 W(J) = 0.0
      W(1) = N
      DO 6  J=1,LZ
    6 Z(J) = 0.0
      DO 16  I =1,N
      P = 1.0
      Z(1) = Z(1)+Y(I)
      DO 13  J=2,LZ
      P = X(I)*P
      W(J) = W(J)+P
   13 Z(J) = Z(J)+Y(I)*P
      DO 16  J=LB,LW
      P = X(I)*P
   16 W(J) = W(J)+P

C
```

SUBROUTINE LEASQ ...(CONT'D)

```
      DO 20  I=1,LZ
      DO 20  K=1,LZ
      J = K+I
   20 B(K,I) = W(J-1)
      DO 22  K=1,LZ
   22 B(K,LB) = Z(K)
      DO 31 L=1,LZ
      DIVB = B(L,L)
      DO 26  J=L,LB
   26 B(L,J) = B(L,J)/DIVB
      I1 = L+1
      IF (I1-LB) 28,33,33
   28 DO 31  I=I1,LZ
      FMULT  = B(I,L)
      DO 31  J=L,LB
   31 B(I,J) = B(I,J)-B(L,J)*FMULT
   33 A(LZ) = B(LZ,LB)
      I = LZ
C         CALCULATE THE POLYNOMIAL COEFFICIENTS
   35 SIGMA = 0.0
      DO 37  J=I,LZ
   37 SIGMA = SIGMA+B(I-1,J)*A(J)
      I = I-1
      A(I) = B(I,LB)-SIGMA
      IF (I-1) 41,41,35
   41 CONTINUE
      RETURN
      END
```

SUBROUTINE QSF

```
      SUBROUTINE  QSF  (H,Y,Z,NDIM)
C
C
C                    SUBROUTINE  QSF
C                    ---------------
C
C
C     PURPOSE
C        COMPUTE THE VECTOR OF INTEGRAL VALUES FOR A GIVEN
C        EQUIDISTANT TABLE OF FUNCTION VALUES
C
C     DESCRIPTION OF PARAMETERS
C        H      -   INCREMENT OF ARGUMENT VALUES
C        Y          INPUT VECTOR OF FUNCTION VALUES
C        Z          RESULTING VECTOR OF INTEGRAL VALUES
C                   Z MAY BE IDENTICAL TO Y
C        NDIM       DIMENSIONS OF VECTOR Y AND Z
C
C     USAGE
C        CALL QSF(H,Y,Z,NDIM)
C
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C        NONE
C
C     REMARKS
C        NO ACTION IN CASE NDIM IS LESS THAN 3
C        THIS SUBROUTINE IS WRITTEN BY IBM (IBM/1130 S.S.P.)
C
C

      DIMENSION Y(6),Z(5)
      HT=.3333333*H
      IF(NDIM-5)7,8,1

C     NDIM IS GREATER THAN 5. PREPARATIONS OF INTEGRATION
C     LOOP

    1 SUM1=Y(2)+Y(2)
      SUM1=SUM1+SUM1
      SUM1=HT*(Y(1)+SUM1+Y(3))
      AUX1=Y(4)+Y(4)
      AUX1=AUX1+AUX1
      AUX1=SUM1+HT*(Y(3)+AUX1+Y(5))
      AUX2=HT*(Y(1)+3.875*(Y(2)+Y(5))+2.625*(Y(3)+Y(4))
     *+Y(6))
      SUM2=Y(5)+Y(5)
      SUM2=SUM2+SUM2
      SUM2=AUX2-HT*(Y(4)+SUM2+Y(6))
```

SUBROUTINE QSF ...(CONT'D)

```
      Z(1)=0.
      AUX=Y(3)+Y(3)
      AUX=AUX+AUX
      Z(2)=SUM2-HT*(Y(2)+AUX+Y(4))
      Z(3)=SUM1
      Z(4)=SUM2
      IF(NDIM-6)5,5,2
C
C     INTEGRATION LOOP
C
    2 DO 4 I=7,NDIM,2
      SUM1=AUX1
      SUM2=AUX2
      AUX1=Y(I-1)+Y(I-1)
      AUX1=AUX1+AUX1
      AUX1=SUM1+HT*(Y(I-2)+AUX1+Y(I))
      Z(I-2)=SUM1
      IF(I-NDIM)3,6,6
    3 AUX2=Y(I)+Y(I)
      AUX2=AUX2+AUX2
      AUX2=SUM2+HT*(Y(I-1)+AUX2+Y(I+1))
    4 Z(I-1)=SUM2
    5 Z(NDIM-1)=AUX1
      Z(NDIM)=AUX2
      RETURN
    6 Z(NDIM-1)=SUM2
      Z(NDIM)=AUX1
      RETURN
C
C     END OF INTEGRATION LOOP
C
    7 IF(NDIM-3)12,11,8
C
C     NDIM IS EQUAL TO 4 OR 5
C
    8 SUM2=1.125*HT*(Y(1)+Y(2)+Y(2)+Y(2)+Y(3)+Y(3)+Y(3)
     *+Y(4))
      SUM1=Y(2)+Y(2)
      SUM1=SUM1+SUM1
      SUM1=HT*(Y(1)+SUM1+Y(3))
      Z(1)=0.
      AUX1=Y(3)+Y(3)
      AUX1=AUX1+AUX1
      Z(2)=SUM2-HT*(Y(2)+AUX1+Y(4))
      IF(NDIM-5)10,9,9
    9 AUX1=Y(4)+Y(4)
      AUX1=AUX1+AUX1
      Z(5)=SUM1+HT*(Y(3)+AUX1+Y(5))
   10 Z(3)=SUM1
      Z(4)=SUM2
```

SUBROUTINE QSF ...(CONT'D)

```
      RETURN
C     NDIM IS EQUAL TO 3
   11 SUM1=HT*(1.25*Y(1)+Y(2)+Y(2)-.25*Y(3))
      SUM2=Y(2)+Y(2)
      SUM2=SUM2+SUM2
      Z(3)=HT*(Y(1)+SUM2+Y(3))
      Z(1)=0.
      Z(2)=SUM1
   12 RETURN
      END
```

MAINLINE FDLOO

```
      MAINLINE FDLOO
C
C
C          *************************
C          *                       *
C          *    MAINLINE  FDLOO    *
C          *    ---------------    *
C          *                       *
C          *************************
C
C
C     PURPOSE
C        FIT THE FREQUENCY RESPONSE DATA BY AN ALGEBRAIC
C        EXPRESSION USING LEVY'S CURVE FITTING METHOD
C        THE FORM OF THE EXPRESSION IS THAT OF A RATIO OF
C        TWO
C        FREQUENCY-DEPENDENT POLYNOMIALS
C
C            A(0)+A(1)*W+A(2)*W**2+A(3)*W**3+...
C        G = -----------------------------------
C            B(0)+B(1)*W+B(2)*W**2+B(3)*W**3+...
C        WITH  B(0) = 1.0
C
C     DESCRIPTION OF PARAMETERS
C        NDATA     NUMBER OF DATA CARDS OF EACH SET TO BE
C                  READ IN
C        NFQ       NUMBER OF DATA POINTS TO BE USED IN THE
C                  CALCULATIONS
C        AMAG      MAGNITUDE
C        OMEGA     FREQUENCY
C        PH        PHASE SHIFT (EITHER IN DEGREES OR IN
C                  RADIANS)
C        AREAL     REAL COMPONENT OF THE MAGNITUDE RATIO
C        AIMAG     IMAGINARY COMPONENT OF THE MAGNITUDE
C                  RATIO
C        NUM       ORDER OF THE NUMERATOR OF THE POLYNOMIAL
C        NDE       ORDER OF THE DENOMINATOR OF THE
C                  POLYNOMIAL
C        INDEX     DUMMY ARGUMENT WHICH IS EQUAL TO
C                  0 IF GIVEN PHASE LAGS ARE IN RADIANS
C                  1 IF GIVEN PHASE LAGS ARE IN DEGREES
C        NCASE     NUMBER OF CASES STUDIED
C
C     USAGE
C        ENTER DATA AS REQUIRED
C
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C        SOLEQ, SECTF
C        LISTINGS OF SUBROUTINE SOLEQ APPEAR ON PAGE B- 42
```

MAINLINE FDL00 ...(CONT'D)

```
C
C     METHOD
C        COMPLEX CURVE FITTING
C
C     REFERENCE
C        LEVY, E.C., 'COMPLEX CURVE FITTING', INSTITUTE OF
C        RADIO ENGINEERE
C        RADIO ENGINEERS, TRANS. ON AUTOMATIC CONTROL, VOL.
C        AC-4, PP. 37-43, MAY, 1966.
C
C     REMARKS
C        THIS METHOD IS RESTRICTED TO SYSTEMS HAVING A
C        FINITE  MAGNITUDE
C        AT ZERO FREQUENCY
C
C

      DIMENSION OMEGA(50),AMAG(50),PHASE(50),PH(50),AMAT(50)
      DIMENSION ALAMD(20),SSS(20),TTT(20),UUU(20),RES(20),
     1A(10,20),C(20,1)
      DIMENSION AREAL(50),AIMAG(50)
      DIMENSION TITLE(15)
      READ (5,15) NCASE
   15 FORMAT (I5)
      DO 444 JKL=1,NCASE
      READ (5,579)(TITLE(I),I=1,15)
  579 FORMAT (15A4)
      READ (5,1) NDATA,NFQ,INDEX
    1 FORMAT (3I5)
      READ (5,2) (OMEGA(IW),AMAT(IW),PH(IW),IW=1,NDATA)
    2 FORMAT (5X,F14.4,14X,F11.3,F14.3)

C        COMPUTE THE AMPLITUDE RATIOS - NORMALIZE THE
C        MAGNITUDES OF THE BODE PLOT

      DO 4443  IW=1,NFQ
      AMAG(IW) = AMAT(IW)/AMAT(1)
 4443 CONTINUE

C        READ ORDERS OF THE NUMERATOR AND THE DENOMINATOR OF
C        THE TRANSFER FUNCTION

      READ (5,3) NUM,NDE
    3 FORMAT (2I5)
      IF(INDEX-1) 500,502,500
  500 CONTINUE
      DO 501  IW=1,NFQ
      PHASE(IW) = PH(IW)
  501 CONTINUE
      GO TO 503
```

```
  502 CONTINUE
C         CONVERSION PHASE LAGS FROM DEGREES TO RADIANS
      PI = 3.14159265
      DO 503  IW=1,NFQ
      PHASE(IW) = PH(IW)*PI/180.0
  503 CONTINUE
C         CALCULATE REAL AND IMAGINARY COMPONENTS OF
C         AMPLITUDE RATIOS
      DO 504  IW=1,NFQ
      AREAL(IW) = AMAG(IW)*COS(PHASE(IW))
      AIMAG(IW) = AMAG(IW)*SIN(PHASE(IW))
  504 CONTINUE

      NUMP = NUM+1
      NUMDE = NUMP+NDE
      NUMD2 = NUMDE*NUMDE
      NUMP1 = NUMP+1
      NUMP2 = NUMP+2
      NDEE = NDE*2
      NUMPP = NUMP*2

      WRITE (6,582)
  582 FORMAT (1H1////)
      WRITE (6,577) (TITLE(I),I=1,15)
  577 FORMAT (15A4)
C         EVALUATE LAMDA(I) , S(I) , T(I) , U(I)
      ALAMD(1) = FLOAT(NFQ)
      DO 1000  I=3,NUMPP,2
      ALAMD(I) = 0.0
      DO 1000  IW=1,NFQ
      ALAMD(I) = ALAMD(I)+OMEGA(IW)**(I-1)
 1000 CONTINUE
      DO 1001  I=1,NUMDE,2
      K = I+1
      TTT(I) = 0.0
      SSS(K) = 0.0
      DO 1001  IW=1,NFQ
      TTT(I) = TTT(I)+AIMAG(IW)*OMEGA(IW)**I
      SSS(K) = SSS(K)+AREAL(IW)*OMEGA(IW)**K
 1001 CONTINUE
      SOO = 0.0
      DO 2500  IW=1,NFQ
```

MAINLINE FDLOO ...(CONT'D)

```
      SOO = SOO+AREAL(IW)
 2500 CONTINUE
      DO 1002  I=2,NDEE,2
      UUU(I) = 0.0
      DO 1002  IW=1,NFQ
      UUU(I) = UUU(I)+(AREAL(IW)*AREAL(IW)+AIMAG(IW)
     **AIMAG(IW))*
     1OMEGA(IW)**I
 1002 CONTINUE

C         EVALUATE ALL ELEMENTS OF COLUMN MATRIX C

      C(1,1) = SOO
      DO 2501  I=2,NUMP,2
      IM1 = I-1
      C(I,1) = TTT(IM1)
 2501 CONTINUE
      DO 2504  I=3,NUMP,2
      IM1 = I-1
      C(I,1) = SSS(IM1)
 2504 CONTINUE
      DO 2502  I=NUMP1,NUMDE,2
      C(I,1) = 0.0
 2502 CONTINUE
      DO 2503  I=NUMP2,NUMDE,2
      KSI = I-NUMP
      C(I,1) = UUU(KSI)
 2503 CONTINUE

C         EVALUATE ALL ELEMENTS OF MATRIX A
C
C         INITIALLY , SET ALL ELEMENTS OF MATRIX A EQUAL TO 0

      DO 1900  I=1,NUMDE
      DO 1900  J=1,NUMDE
      A(I,J) = 0.0
 1900 CONTINUE

C         ARRANGE ALL ELEMENTS OF UPPER LEFT CORNER OF MATRIX
C         A

      DO 2000  I=1,NUMP,2
      DO 2000  J=1,NUMP,2
      KJ = (J-1)/2
      KT = I+J-1
      A(I,J) = ALAMD(KT)*(-1)**KJ
 2000 CONTINUE
      DO 2001  I=2,NUMP,2
      DO 2001  J=2,NUMP,2
      KJ = J/2-1
```

MAINLINE FDLOO ...(CONT'D)

```
      KT = I+J-1
      A(I,J) = ALAMD(KT)*(-1)**KJ
 2001 CONTINUE
C
C        ARRANGE ALL ELEMENTS OF UPPER RIGHT CORNER OF
C        MATRIX A
C
      DO 2002  I=1,NUMP,2
      DO 2002  J=NUMP1,NUMDE,2
      KSJ = J-NUMP
      KJ = (KSJ-1)/2
      KT = I+KSJ-1
      A(I,J) = TTT(KT)*(-1)**KJ
 2002 CONTINUE
      DO 2003  I=2,NUMP,2
      DO 2003  J=NUMP1,NUMDE,2
      KSJ = J-NUMP
      KJ = (KSJ+1)/2
      KT = I+KSJ-1
      A(I,J) = SSS(KT)*(-1)**KJ
 2003 CONTINUE
      DO 2004  I=1,NUMP,2
      DO 2004  J=NUMP2,NUMDE,2
      KSJ = J-NUMP
      KJ = KSJ/2-1
      KT = I+KSJ-1
      A(I,J) = SSS(KT)*(-1)**KJ
 2004 CONTINUE
      DO 2005  I=2,NUMP,2
      DO 2005  J=NUMP2,NUMDE,2
      KSJ = J-NUMP
      KJ = KSJ/2-1
      KT = I+KSJ-1
      A(I,J) = TTT(KT)*(-1)**KJ
 2005 CONTINUE
C
C        ARRANGE ALL ELEMENTS OF LOWER LEFT CORNER OF MATRIX
C        A
C
      DO 2006  I=NUMP1,NUMDE,2
      DO 2006  J=1,NUMP,2
      KSI = I-NUMP
      KJ = (J-1)/2
      KT = KSI+J-1
      A(I,J) = TTT(KT)*(-1)**KJ
 2006 CONTINUE
      DO 2007  I=NUMP1,NUMDE,2
      DO 2007  J=2,NUMP,2
      KSI = I-NUMP
      KJ = J/2
```

```
      KT = KSI+J-1
      A(I,J) = SSS(KT)*(-1)**KJ
 2007 CONTINUE
      DO 2008  I=NUMP2,NUMDE,2
      DO 2008  J=1,NUMP,2
      KSI = I-NUMP
      KJ = (J-1)/2
      KT = KSI+J-1
      A(I,J) = SSS(KT)*(-1)**KJ
 2008 CONTINUE
      DO 2009  I=NUMP2,NUMDE,2
      DO 2009  J=2,NUMP,2
      KSI = I-NUMP
      KJ = J/2-1
      KT = KSI+J-1
      A(I,J) = TTT(KT)*(-1)**KJ
 2009 CONTINUE

C         ARRANGE ALL ELEMENTS OF LOWER RIGHT CORNER OF
C         MATRIX A

      DO 2010  I=NUMP1,NUMDE,2
      DO 2010  J=NUMP1,NUMDE,2
      KSI = I-NUMP
      KSJ = J-NUMP
      KJ = (KSJ-1)/2
      KT = KSI+KSJ
      A(I,J) = UUU(KT)*(-1)**KJ
 2010 CONTINUE
      DO 2011  I=NUMP2,NUMDE,2
      DO 2011  J=NUMP2,NUMDE,2
      KSI = I-NUMP
      KSJ = J-NUMP
      KJ = KSJ/2-1
      KT = KSI+KSJ
      A(I,J) = UUU(KT)*(-1)**KJ
 2011 CONTINUE
      DO 2350  I=NUMP1,NUMDE,2
      DO 2350  J=NUMP2,NUMDE,2
      A(I,J) = 0.0
 2350 CONTINUE
      DO 2355  I=NUMP2,NUMDE,2
      DO 2355  J=NUMP1,NUMDE,2
      A(I,J) = 0.0
 2355 CONTINUE

C         SOLVE THESE EQUATIONS USING SUBROUTINE SOLEQ

      CALL SOLEQ (A,C,NUMDE,1,DET,-1)
```

MAINLINE FDL00 ...(CONT'D)

```
C         THE SOLUTIONS WILL BE STORED IN THE MATRIX RES

      DO 2100  I=1,NUMDE
      RES(I) = C(I,1)
 2100 CONTINUE


      WRITE (6,9100)
 9100 FORMAT (///10X,'TRANSFER FUNCTION COEFFICIENTS IN THE
     * NUMERATOR')
      DO 9101 I=1,NUMP
      K = I-1
      WRITE (6,9102) K,RES(I)
 9102 FORMAT (1H0,12X,'A (',I2,') =',E12.5)
 9101 CONTINUE
      WRITE (6,9103)
 9103 FORMAT (///10X,'TRANSFER FUNCTION COEFFICIENTS IN THE
     * DENOMINATOR'
     1)
      WRITE (6,9106)
 9106 FORMAT (1H0,12X,'B ( 0) = 0.10000E 01')
      DO 9104   I=NUMP1,NUMDE
      J = I-NUMP
      WRITE (6,9105) J,RES(I)
 9105 FORMAT (1H0,12X,'B (',I2,') =',E12.5)
 9104 CONTINUE

C         IF THE MODEL IS A SECOND ORDER TRANSFER FUNCTION ,
C         CALCULATE TAU1 , TAU2 , AND THE GAIN

      IF(NUM) 9001,9000,9001
 9000 CONTINUE
      IF(NDE-2) 9001,9003,9001
 9003 CONTINUE
      CALL SECTF(RES)
 9001 CONTINUE
  444 CONTINUE
      CALL EXIT
      END
```

SUBROUTINE SECTF

```
      SUBROUTINE SECTF(RES)
C
C
C                    SUBROUTINE  SECTF
C                    -----------------
C
C
C     PURPOSE
C        CALCULATE THE GAIN, TAU1, TAU2 OF A SECOND ORDER
C        TRANSFER FUNCTION FROM THE PARAMETERS GIVEN BY THE
C        GENERAL EXPRESSION OF THE TRANSFER FUNCTION
C
C     DESCRIPTION OF PARAMETERS
C        RES         PARAMETERS GIVEN BY THE GENERAL
C                    EXPRESSION OF THE TRANSFER FUNCTION WHERE
C        A0          RES(1)
C        B1          RES(2)
C        B2          RES(3)
C
C     USAGE
C        CALL SECTF(RES)
C
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C        NONE
C
C

      DIMENSION RES(20)
      A0 = RES(1)
      B1 = RES(2)
      B2 = RES(3)
      DELTA = B1*B1-4.0*B2
      IF(DELTA) 1,2,2

C        THE TRANSFER FUNCTION IS UNDERDAMPED - RETURN

    1 CONTINUE
      RETURN

C        THE TRANSFER FUNCTION IS OF THE FORM OF TWO FIRST
C        ORDER IN SERIES

    2 CONTINUE
      WRITE (6,20)
   20 FORMAT (1H1)
      WRITE (6,10)
   10 FORMAT (///10X,'SECOND ORDER TRANSFER FUNCTION
     * REPRESENTATION')
      TAUA1 = (B1+SQRT(DELTA))/2.0
```

SUBROUTINE SECTF ...(CONT'D)

```
      TAUB1 = (B1-SQRT(DELTA))/2.0
      WRITE (6,15) TAUA1,TAUB1
   15 FORMAT (1H0,12X,'TAU1 =',E12.5, 10X,'TAU2 =',E12.5)
      RETURN
      END
```

MAINLINE FDSSO

```
      MAINLINE FDSSO
C
C
C           *************************
C           *                       *
C           *    MAINLINE  FDSSO    *
C           *    ---------------    *
C           *                       *
C           *************************
C
C
C     PURPOSE
C        DETERMINE THE TRANSFER FUNCTION COEFFICIENTS FROM
C        FREQUENCY DOMAIN DATA USING STAFFIN AND STAFFIN'S
C        METHOD
C
C        THE FORM OF THE EXPRESION OF THE TRANSFER FUNCTION
C        IS THAT OF A RATIO OF TWO FREQUENCY-DEPENDENT POLY-
C        NOMIALS SUCH AS DESCRIBED BY EQUATION (4.3-1B) OF
C        THE AUTHOR'S THESIS I.E.
C
C            B(0)+B(1)*W+B(2)*W**2+B(3)*W**3+...
C        G = -----------------------------------
C            A(0)+A(1)*W+A(2)*W**2+A(3)*W**3+...
C        WITH A(0) = 1.0
C
C     DESCRIPTION OF PARAMETERS
C        NFQ        NUMBER OF DATA POINTS
C        NOPT       INTEGERS WHICH DETERMINE HOW MANY DATA
C                   POINTS TO BE SKIPPED FOR EVERY DATA POINT
C                   USED IN THE CALCULATIONS
C        OMEGA      FREQUENCY
C        PH         PHASE SHIFT (EITHER IN DEGREES OR IN
C                   RADIANS)
C        AREAL      REAL COMPONENT OF THE MAGNITUDE RATIO
C        AIMAG      IMAGINARY COMPONENT OF THE MAGNITUDE
C                   RATIO
C        NUM        ORDER OF THE NUMERATOR OF THE POLYNOMIAL
C        NDE        ORDER OF THE DENOMINATOR OF THE
C                   POLYNOMIAL
C        INDEX      DUMMY ARGUMENT WHICH IS EQUAL TO
C                   0 IF GIVEN PHASE LAGS ARE IN RADIANS
C                   1 IF GIVEN PHASE LAGS ARE IN DEGREES
C        NCASE      NUMBER OF CASES STUDIED
C
C     USAGE
C        ENTER DATA AS REQUIRED
C
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
```

```
C         SECTF, SOLEQ
C         LISTINGS OF SUBROUTINE SOLEQ APPEAR ON PAGE B- 42
C
C      METHOD
C         STAFFIN AND STAFFIN'S METHOD
C
C      REFERENCE
C         STAFFIN, H.K., AND STAFFIN, R., 'APPROXIMATING
C         TRANSFER FUNCTIONS FROM FREQUENCY RESPONSE DATA',
C         INSTRUMENTS AND CONTROL SYSTEMS, VOL. 38, PP.
C         137-144, FEB. 1965.
C
C
C      REMARKS
C         THIS METHOD IS RESTRICTED TO SYSTEMS HAVING A
C         FINITE  MAGNITUDE
C         AT ZERO FREQUENCY
C
C

      DIMENSION AREAL(50), AIMAG(50)
      DIMENSION ADUM(50,5)
      DIMENSION OMEGA(50),AMAG(50),PHASE(50),PH(50)
      DIMENSION DAT(10,20), RES(20), C(10,10)
      DIMENSION AMAT (50)
      DIMENSION TITLE(15)
      READ (5,15) NCASE
   15 FORMAT (I5)
      DO 444 JKL=1,NCASE
      READ (5,579)(TITLE(I),I=1,15)
  579 FORMAT (15A4)
      READ (5,1) NFQ,NOPT,INDEX
    1 FORMAT (3I5)
      READ (5,2) (OMEGA(IW),AMAT(IW),PH(IW),IW=1,NFQ)
    2 FORMAT (5X,F14.4,14X,F11.3,F14.3)
C         NORMALIZE AMPLITUDE RATIOS
C
      DO 4443  IW=1,NFQ
      AMAG(IW) = AMAT(IW)/AMAT(1)
 4443 CONTINUE
C         READ ORDERS OF THE NUMERATOR AND THE DENOMINATOR OF
C         THE
C         TRANSFER FUNCTION
C
      READ (5,3) NUM,NDE
    3 FORMAT (2I5)
```

```
      IF(INDEX-1) 500,502,500
  500 CONTINUE
      DO 501  IW=1,NFQ
      PHASE(IW) = PH(IW)
  501 CONTINUE
      GO TO 503
  502 CONTINUE
C
C        CONVERT PHASE LAGS FROM DEGREES TO RADIANS

      PI = 3.14159265
      DO 503  IW=1,NFQ
      PHASE(IW) = PH(IW)*PI/180.0
  503 CONTINUE

C        CALCULATE REAL AND IMAGINARY COMPONENTS OF
C        AMPLITUDE RATIOS

      DO 504  IW=1,NFQ
      AREAL(IW) = AMAG(IW)*COS(PHASE(IW))
      AIMAG(IW) = AMAG(IW)*SIN(PHASE(IW))
  504 CONTINUE


      NDEP1 = NDE+1
      NDEP2 = NDE+2
      NTOTL = NUM+NDE+1

C        SET UP THE COEFFICIENTS FOR MATRIX DAT

      NTOTV = NTOTL*NOPT
      DO 1500  IW=1,NTOTV,NOPT
      IV = IW/NOPT+1
      ADUM(IW,1) =  AREAL(IW)+AIMAG(IW)
      ADUM(IW,2) =  AREAL(IW)-AIMAG(IW)
      ADUM(IW,3) = -AREAL(IW)-AIMAG(IW)
      ADUM(IW,4) = -AREAL(IW)+AIMAG(IW)
      DO 1100  J=2,NDEP1
      JJ = J/4
      ISIGN = J-JJ*4
      IF (ISIGN) 1030,1050,1030
 1050 CONTINUE
      ISIGN = 4
 1030 CONTINUE
      L = J-1
      DAT(IV,L) = ADUM(IW,ISIGN)*OMEGA(IW)**(J-1)
 1100 CONTINUE
      DO 1200  J=NDEP1,NTOTL
      NDUM = J-NDEP1
```

```
      DAT(IV,J) = -OMEGA(IW)**NDUM
 1200 CONTINUE
 1500 CONTINUE
      DO 1600  IW=1,NTOTV,NOPT
      IV = IW/NOPT+1
      C(IV,1) = -AREAL(IW)-AIMAG(IW)
 1600 CONTINUE
      CALL SOLEQ (DAT,C,NTOTL,1,DET,-1)
      DO 2100  I=1,NTOTL
      RES(I) = C(I,1)
 2100 CONTINUE


      WRITE (6,9103)
 9103 FORMAT (///10X,'TRANSFER FUNCTION COEFFICIENTS IN THE
     * DENOMINATOR'
     1)
      WRITE (6,8889)
 8889 FORMAT (1H0,12X,'A ( 0) = 0.10000E 01')
      DO 9101 I=1,NDE
      K = I
      WRITE (6,9102) K,RES(I)
 9102 FORMAT (1H0,12X,'A (',I2,') =',E12.5)
 9101 CONTINUE
      WRITE (6,9100)
 9100 FORMAT (///10X,'TRANSFER FUNCTION COEFFICIENTS IN THE
     * NUMERATOR')
      DO 9104  I=NDEP1,NTOTL
      J = I-NDEP1
      WRITE (6,9105) J,RES(I)
 9105 FORMAT (1H0,12X,'B (',I2,') =',E12.5)
 9104 CONTINUE

C
C        IF THE MODEL IS THAT OF TWO FIRST ORDER TRANSFER
C        FUNCTIONS IN SERIES, DETERMINE THE GAIN, TAU1 AND
C        TAU2

      IF(NUM) 9001,9000,9001
 9000 CONTINUE
      IF(NDE-2) 9001,9003,9001
 9003 CONTINUE
      CALL SECTB(RES)
 9001 CONTINUE
  444 CONTINUE
      CALL EXIT
      END
```

SUBROUTINE SECTB

```
      SUBROUTINE SECTB(RES)
C
C
C                  SUBROUTINE  SECTB
C                  -----------------
C
C
C     PURPOSE
C        CALCULATE THE GAIN, TAU1, TAU2 OF A SECOND ORDER
C        TRANSFER FUNCTION FROM THE PARAMETERS GIVEN BY THE
C        GENERAL EXPRESSION OF THE TRANSFER FUNCTION
C
C     DESCRIPTION OF PARAMETERS
C        RES        PARAMETERS GIVEN BY THE GENERAL
C                   EXPRESSION OF THE TRANSFER FUNCTION WHERE
C        B1         RES(1)
C        B2         RES(2)
C        A0         RES(3)
C
C     USAGE
C        CALL SECTB(RES)
C
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C        NONE
C
C

      DIMENSION RES(20)
      B1 = RES(1)
      B2 = RES(2)
      A0 = RES(3)
      DELTA = B1*B1-4.0*B2
      IF(DELTA) 1,2,2

C         THE TRANSFER FUNCTION IS UNDERDAMPED - RETURN

    1 CONTINUE
      RETURN
    2 CONTINUE

C         THE TRANSFER FUNCTION IS OF THE FORM OF TWO FIRST
C         ORDER IN SERIES

      WRITE (6,20)
   20 FORMAT (1H1)
      WRITE (6,10)
   10 FORMAT (///10X,'SECOND ORDER TRANSFER FUNCTION
     * REPRESENTATION')
      TAUA1 = (B1+SQRT(DELTA))/2.0
```

SUBROUTINE SECTB ...(CONT'D)

```
      TAUB1 = (B1-SQRT(DELTA))/2.0
      WRITE (6,15) TAUA1,TAUB1
   15 FORMAT (1H0,12X,'TAU1 =',E12.5,10X,'TAU2 =',E12.5)
      RETURN
      END
```

MAINLINE FDROO

```
      MAINLINE FDROO
C
C
C                 ***************************
C                 *                         *
C                 *     MAINLINE  FDROO     *
C                 *     ---------------     *
C                 *                         *
C                 ***************************
C
C
C     PURPOSE
C        FIT THE FREQUENCY-DOMAIN DATA BY SIMPLE TRANSFER
C        FUNCTIONS USING ROSENBROCK'S SEARCH TECHNIQUES
C
C     DESCRIPTION OF PARAMETERS
C        NVAR      NUMBER OF PARAMETERS TO BE OPTIMIZED
C        M         PROGRAM CONTROL FLAG
C                   1 ... MAXIMIZE A FUNCTION
C                  -1 ... MINIMIZE A FUNCTION
C        CONVC     BASE POINT CONVERGENCE RATIO
C        ACONS     LOWER LIMITS FOR THE PARAMETERS
C        UCONS     UPPER LIMITS FOR THE PARAMETERS
C        B1        STARTING POINT
C        STEPS     INITIAL STEP SIZE FOR THE PARAMETERS
C        NFQ       NUMBER OF DATA POINTS TO BE USED IN THE
C                  CALCULATIONS
C        OMEGA     FREQUENCY
C        AMAG      MAGNITUDE OF THE BODE PLOT
C        TAU1      MINOR TIME CONSTANT
C        TAU2      MAJOR TIME CONSTANT
C        NCASE     NUMBER OF CASES STUDIED
C
C     USAGE
C        ENTER DATA AS REQUIRED
C
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C        RBRCK, ADVCE, CONTR, SOLNS, FUNC
C        LISTINGS OF SUBROUTINE RBRCK APPEAR ON PAGE B-  9
C        LISTINGS OF SUBROUTINE ADVCE APPEAR ON PAGE B- 15
C        LISTINGS OF SUBROUTINE CONTR APPEAR ON PAGE B- 16
C        LISTINGS OF SUBROUTINE SOLNS APPEAR ON PAGE B- 18
C
C
      COMMON AXES(5,5),B1(5),B2(5),UCONS(5),ACONS(5),A(5,5)
     *,B(5),
     1STEPS(5),BASE,BNEW,SUM,CONVC,AM(5),AJUMP,IFL(5),NVAR,M
     *,SNEW
```

MAINLINE FDROO ...(CONT'D)

```
      DIMENSION AMAG(100)
      COMMON/ALEAS/Y(100),OMEGA(100),NPTS,SUMSQ
C        READ IN DATA
      READ (5,1) NVAR,M
    1 FORMAT (2I5)
      READ (5,3) CONVC
    3 FORMAT (F10.8)
      READ (5,2) (B1(I),I=1,5)
    2 FORMAT (5F10.5)
      READ (5,4) (ACONS(I),I=1,5)
      READ (5,4) (UCONS(I),I=1,5)
      READ (5,4) (STEPS(I),I=1,5)
    4 FORMAT (5F10.3)
      READ (5,10) NCASE
   10 FORMAT (I5)
      DO 9999  ICASE=1,NCASE
C        READ IN FREQUENCY RESPONSE DATA
      READ (5,7) NFQ
    7 FORMAT (I5)
      NPTS = NFQ
      READ (5,100) (OMEGA(I),AMAG(I),I=1,40)
  100 FORMAT (10X,F9.4,17X,F9.4)
C        WRITE OUT INPUT DATA
      WRITE (6,50)
   50 FORMAT(1H1,20X,'ROSENBROCK S SEARCH TECHNIQUE'/21X,'--
     *------------
     1---------------'//)
      WRITE (6,51) NVAR
   51 FORMAT (1H0,10X,'DIMENSIONS OF SPACE ',I3)
      WRITE (6,52) M
   52 FORMAT (1H0,10X,'CRITERION - MAXIMIZE (+1) , MINIMIZE
     * (-1)',I5)
      WRITE (6,53) CONVC
   53 FORMAT (1H0,10X,'BASE POINT CONVERGENCE RATIO',F14.8)
      WRITE (6,54)
   54 FORMAT (///11X,'INITIAL BASE POINT')
      WRITE (6,55) (B1(I),I=1,NVAR)
      WRITE (6,56)
   56 FORMAT (///11X, 'BASIC STEP SIZES')
      WRITE (6,55) (STEPS(I),I=1,NVAR)
      WRITE (6,57)
   57 FORMAT (///11X,'UPPER CONSTRAINTS')
      WRITE (6,55) (UCONS(I),I=1,NVAR)
      WRITE (6,58)
```

MAINLINE FDROO ...(CONT'D)

```
   58 FORMAT (///11X,'LOWER CONSTRAINTS')
      WRITE (6,55) (ACONS(I),I=1,NVAR)
   55 FORMAT (15X,F12.5)
      WRITE (6,70)
   70 FORMAT (1H1)
C
C         CALCULATE THE AMPLITUDE RATIOS
C
      DO 3510  I=1,NPTS
      Y(I) = AMAG(I)/AMAG(1)
 3510 CONTINUE
      WRITE (6,123) (OMEGA(I),AMAG(I),Y(I),I=1,NPTS)
  123 FORMAT (1H ,3E18.6)
C
C         MINIMIZE THE FUNCTION VALUE
C
      CALL RBRCK
      TAU1 = B2(1)
      TAU2 = B2(2)
C
C         WRITE OUT THE RESULTS
C
      WRITE (6,61)
   61 FORMAT (///27X,'PROCESS PARAMETERS'/27X,'-------------
     *-----'//)
      WRITE (6,62) TAU1,TAU2
   62 FORMAT (1H0,20X,'TAU1 =',F15.3,7X,'TAU2 =',F15.3)
 9999 CONTINUE
      CALL EXIT
      END
```

FUNCTION FUNC

```
      FUNCTION FUNC (NVAR,B2)
C
C
C                       FUNCTION  FUNC
C                       --------------
C
C
C     PURPOSE
C        COMPUTE THE VALUE OF THE FUNCTION TO BE OPTIMIZED
C        THE MODEL IS THAT OF TWO FIRST ORDER TRANSFER
C        FUNCTIONS IN SERIES
C
C     DESCRIPTION OF PARAMETERS
C        NVAR     NUMBER OF PARAMETERS TO BE OPTIMIZED
C        B2       VALUES OF THE RESPECTIVE PARAMETERS
C
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C        NONE
C
C
      COMMON/ALEAS/Y(100),OMEGA(100),NPTS,SUMSQ
      DIMENSION B2(5)
      TAU1 = B2(1)
      TAU2 = B2(2)
      SUMSQ = 0.0
      DO 100  I=1,NPTS
      TERM1 = TAU1*TAU1*OMEGA(I)*OMEGA(I)+1.0
      TERM2 = TAU2*TAU2*OMEGA(I)*OMEGA(I)+1.0
      AMODL = 1.0/SQRT(TERM1*TERM2)
      SUMSQ = SUMSQ+(Y(I)-AMODL)**2
  100 CONTINUE
      FUNC = SUMSQ
      RETURN
      END
```

APPENDIX C

LISTINGS OF CSMP PROGRAMS

Since the complete listings of all CSMP programs which have been used during the present investigation would be too voluminous, only some typical S/360 CSMP programs are included in this appendix, namely the control of top product composition by manipulation of reflux flow, the control of the liquid temperature on intermediate tray 8 by manipulation of reflux flow and the control of bottom product composition by manipulation of steam flow using the data as given by the models of the University of Alberta distillation column.

Use of these programs for similar simulation problems necessitates proper modifications of the programs using appropriate data.

```
*                CONTINUOUS SYSTEM MODELING PROGRAM
*                ----------------------------------
*
*
*
*        *********************************************
*        *                                           *
TITLE             CONTROL OF TOP PRODUCT COMPOSITION
*        *                                           *
*        *********************************************
*
*
*  DESCRIPTIONS OF PARAMETERS
*        GDF        TRANSFER FUNCTION OF XD FOR LOAD CHANGES
*        GDM        TRANSFER FUNCTION OF XD FOR CHANGES IN
*                   THE MANIPULATIVE VARIABLE
*        GWF        TRANSFER FUNCTION OF XW FOR LOAD CHANGES
*        GWM        TRANSFER FUNCTION OF XW FOR CHANGES IN
*                   THE MANIPULATIVE VARIABLE
*        ERRES      I.S.E. OF TOP PRODUCT COMPOSITION
*        ERRW2S     I.S.E. OF BOTTOM PRODUCT COMPOSITION
*        AKT        AKC*AKV*AKM
*        AKC        GAIN OF THE FEEDBACK CONTROLLER
*        AKV        GAIN OF THE CONTROL VALVE
*        AKM        GAIN OF THE SENSING ELEMENT
*        AKM        GAIN OF THE SENSING ELEMENT
*        TAUI       INTEGRAL TIME (MIN.)
*        XD         TOP PRODUCT COMPOSITION
*        XW         BOTTOM PRODUCT COMPOSITION
*        FF         LOAD CHANGES
*        SETPT      SET POINT
*
*  USAGE
*        IF FEEDBACK CONTROL ONLY IS DESIRED, SET AKFF = 0.0
*
*  REMARKS
*        SIMULATION USING DATA FROM THE U. OF A. DISTILLATION
*        COLUMN
*

*  DATA REQUIRED FOR THE SIMULATION
*  --------------------------------
*  DATA FOR THE TRANSFER FUNCTION  GDM
PARAMETER     AKDM =  19.730, TAUDM1 = 0.520, TAUDM2 = 27.659
PARAMETER     TDLYDM = 0.000
*  DATA FOR THE TRANSFER FUNCTION  GWM
PARAMETER     AKWM =   4.896, TAUWM1 = 2.717, TAUWM2 = 13.675
PARAMETER     TDLYWM = 4.500
```

```
*  DATA FOR THE TRANSFER FUNCTION  GDF
PARAMETER      AKDF =    6.455, TAUDF1 = 5.143, TAUDF2 = 18.243
PARAMETER      TDLYDF = 3.467
*  DATA FOR THE TRANSFER FUNCTION  GWF
PARAMETER      AKWF =    3.657, TAUWF1 = 0.628, TAUWF2 = 12.889
PARAMETER      TDLYWF = 3.649
*  DATA FOR THE CONTROL VALVE
PARAMETER      AKV  = 1.000
*  DATA FOR THE SENSING ELEMENT FOR TOP PRODUCT COMPOSITION
PARAMETER      AKD  = 1.000
*  DATA FOR THE SENSING ELEMENT OF BOTTOM COMPOSITION
PARAMETER      AKW  = 1.000, TDLYW = 2.500
*  FORCING FUNCTION
PARAMETER      FF   = 0.430
*  SETPOINT
CONSTANT       SETPT = 0.000
*
*  FEEDBACK CONTROLLER CONSTANT
PARAMETER      AKT = 120.0
*  INTEGRAL TIME CONSTANT
PARAMETER      TAUI = 10.0
*  --------------------------------


INITIAL
*  INITIALIZE PROCESS PARAMETERS
         AMEAS   = 0.0


DYNAMIC
*  DYNAMIC SECTION OF THE MODEL
*  DEVIATION FROM SETPOINT
         ERROR   = SETPT-AMEAS
*  PROPORTIONAL CONTROLLER CONSTANT
         AKC     = AKT/(AKV*AKM)
*  FEEDBACK CONTROLLER ( PROPORTIONAL PLUS INTEGRAL )
         CONT    = ERROR+INTGRL(0.0,ERROR/TAUI)
         CONTRL  = AKC*CONT
*  FEEDFORWARD CONTROLLER CONSTANT
         AKGP    = AKDM
         AKGL    = AKDF
         AKFF    = AKGL/(AKGP*AKV)
*  FEEDFORWARD COMPENSATION
         FEEDFD  = -FF*AKFF
*  SIGNAL TO THE VALVE
         SIGNAL  = CONTRL+FEEDFD
*  VALVE OUTPUT
         VALVE   = AKV*SIGNAL
*  DISTURBANCE ON TOP PRODUCT COMPOSITION
         GDF1    = REALPL(0.0,TAUDF1,FF)
```

```
       GDF2     = REALPL(0.0,TAUDF2,GDF1)
       GDF3     = DELAY(13,TDLYDF,GDF2)
       GDF      = GDF3*AKDF
*  CORRECTIVE ACTION ON TOP PRODUCT COMPOSITION
       GDM1     = REALPL(0.0,TAUDM1,VALVE)
       GDM2     = REALPL(0.0,TAUDM2,GDM1)
       GDM      = GDM2*AKDM
*  TOP PRODUCT COMPOSITION
       XD1      = GDF+GDM
       XD       = XD1*AKD
*  MEASUREMENT OF OUTPUT
       AMEAS    = XD*AKD
*  DISTURBANCE ON BOTTOM PRODUCT COMPOSITION
       GWF1     = REALPL(0.0,TAUWF1,FF)
       GWF2     = REALPL(0.0,TAUWF2,GWF1)
       GWF3     = DELAY(14,TDLYWF,GWF2)
       GWF      = GWF3*AKWF
*  CORRECTIVE ACTION ON BOTTOM PRODUCT COMPOSITION
       GWM1     = REALPL(0.0,TAUWM1,VALVE)
       GWM2     = REALPL(0.0,TAUWM2,GWM1)
       GWM3     = DELAY(17,TDLYWM,GWM2)
       GWM      = GWM3*AKWM
*  BOTTOM PRODUCT COMPOSITION
       XWC      = GWF+GWM
       XW1      = DELAY(10,TDLYW,XWC)
       XW       = XW1*AKW
*  DEVIATION OF XW FROM SETPOINT
       ERRW     = SETPT-XWC
*  ERROR DETECTING CIRCUIT
       ERROR2   = ERROR*ERROR
       ERRW2    = ERRW*ERRW
       ERRES    = INTGRL(0.0,ERROR2)
       ERRW2S   = INTGRL(0.0,ERRW2)
TIMER  DELT=0.20, FINTIM=120.0, PRDEL=1.0, OUTDEL=1.0
PRINT  XD,XW,ERRES,ERRW2S
LABEL                 (RD-FB-FF-TAUI=10.0)
PRTPLT XD, XW
END
STOP
ENDJOB
```

```
*            CONTINUOUS SYSTEM MODELING PROGRAM
*            ----------------------------------
*
*
*
*       ****************************************************
*       *                                                  *
TITLE        CONTROL OF THE LIQUID TEMPERATURE ON
TITLE                INTERMEDIATE TRAY 8
*       *                                                  *
*       ****************************************************
*
*
*  DESCRIPTIONS OF PARAMETERS
*       GDF       TRANSFER FUNCTION OF XD FOR LOAD CHANGES
*       GDM       TRANSFER FUNCTION OF XD FOR CHANGES IN
*                 THE MANIPULATIVE VARIABLE
*       GWF       TRANSFER FUNCTION OF XW FOR LOAD CHANGES
*       GWM       TRANSFER FUNCTION OF XW FOR CHANGES IN
*                 THE MANIPULATIVE VARIABLE
*       G8F       TRANSFER FUNCTION OF C8 FOR LOAD CHANGES
*       G8M       TRANSFER FUNCTION OF C8 FOR CHANGES IN
*                 THE MANIPULATIVE VARIABLE
*       ERRW2S    I.S.E. OF BOTTOM COMPOSITION
*       ERRD2S    I.S.E. OF TOP PRODUCT COMPOSITION
*       ERRES     I.S.E. OF THE CONTROLLED VARIABLE
*       XD        TOP PRODUCT COMPOSITION
*       XW        BOTTOM PRODUCT COMPOSITION
*       C8        TEMPERATURE (OR COMPOSITION) OF THE LIQUID
*                 ON TRAY 8
*       AKT       AKC*AKV*AKM
*       AKC       GAIN OF THE FEEDBACK CONTROLLER
*       AKV       GAIN OF THE CONTROL VALVE
*       AKM       GAIN OF THE SENSING ELEMENT
*       TAUI      INTEGRAL TIME (MIN.)
*       FF        LOAD CHANGES
*       SETPT     SET POINT
*
*  USAGE
*       IF FEEDBACK CONTROL ONLY IS DESIRED, SET AKFF = 0.0
*
*  REMARKS
*       SIMULATION USING DATA FROM THE U. OF A. DISTILLATION
*       COLUMN
*
*
*  DATA REQUIRED FOR THE SIMULATION
*  --------------------------------
*  DATA FOR THE TRANSFER FUNCTION  GDM
PARAMETER     AKDM = 19.730, TAUDM1 = 0.520, TAUDM2 = 27.659
PARAMETER     TDLYDM = 0.0
*  DATA FOR THE TRANSFER FUNCTION  GWM
PARAMETER     AKWM = 4.896, TAUWM1 = 2.717, TAUWM2 = 13.675
PARAMETER     TDLYWM = 4.500
```

```
*  DATA FOR THE TRANSFER FUNCTION  G8M
PARAMETER      AK8M = -10.780, TAU8M1 = 0.422, TAU8M2 = 20.569
PARAMETER      TDLY8M = 0.0
*  DATA FOR THE TRANSFER FUNCTION  GDF
PARAMETER      AKDF = 6.455 , TAUDF1 = 5.143 , TAUDF2 = 18.243
PARAMETER      TDLYDF = 3.467
*  DATA FOR THE TRANSFER FUNCTION  GWF
PARAMETER      AKWF = 3.657, TAUWF1 = 0.628, TAUWF2 = 12.889
PARAMETER      TDLYWF = 3.649
*  DATA FOR THE TRANSFER FUNCTION  G8F
PARAMETER      AK8F = -4.078, TAU8F1 = 4.327, TAU8F2 = 13.330
PARAMETER      TDLY8F = 3.467
*  DATA FOR THE CONTROL VALVE
PARAMETER      AKV  = 1.000
*  DATA FOR THE SENSING ELEMENT FOR TOP PRODUCT COMPOSITION
PARAMETER      AKD  = 1.000
*  DATA FOR THE SENSING ELEMENT OF THE TEMPERATURE (OR
*  COMPOSITION) ON INTERMEDIATE TRAY 8
PARAMETER      AKC8 = 1.000
*  DATA FOR THE SENSING ELEMENT OF BOTTOM COMPOSITION
PARAMETER      AKW = 1.000, TDLYW = 2.500
*
*  SETPOINT
CONSTANT       SETPT = 0.0
*
*  FORCING FUNCTION
PARAMETER      FF = 0.430
*
*  FEEDBACK CONTROLLER CONSTANT
PARAMETER      AKT = 224.0
*  INTEGRAL TIME CONSTANT
PARAMETER      TAUI = 10.0
* ------------------------------


INITIAL
*  INITIALIZE PROCESS PARAMETERS
         AMEAS = 0.0


DYNAMIC
*  DYNAMIC SECTION OF THE MODEL
*  DEVIATION FROM SETPOINT
         ERROR   = SETPT+AMEAS
*  PROPORTIONAL CONTROLLER CONSTANT
         AKC     = AKT/(AKV*AKM)
*  FEEDBACK CONTROLLER ( PROPORTIONAL PLUS INTEGRAL )
         CONT    = ERROR+INTGRL(0.0,ERROR/TAUI)
         CONTRL  = AKC*CONT
*  VALVE OUTPUT
         VALVE = AKV*CONTRL
```

```
*  DISTURBANCE ON THE LIQUID TEMPERATURE ON TRAY 8
       G8F1     = REALPL(0.0,TAU8F1,FF)
       G8F2     = REALPL(0.0,TAU8F2,G8F1)
       G8F3     = DELAY(13,TDLY8F,G8F2)
       G8F      = G8F3*AK8F
*  CORRECTIVE ACTION ON THE LIQUID TEMPERATURE ON TRAY 8
       G8M1     = REALPL(0.0,TAU8M1,VALVE)
       G8M2     = REALPL(0.0,TAU8M2,G8M1)
       G8M      = G8M2*AK8M
*  LIQUID TEMPERATURE ON INTERMEDIATE TRAY 8
       C8       = G8F+G8M
*  MEASUREMENT OF OUTPUT
       AMEAS    = C8*AKC8
*  DISTURBANCE ON TOP PRODUCT COMPOSITION
       GDF1     = REALPL(0.0,TAUDF1,FF)
       GDF2     = REALPL(0.0,TAUDF2,GDF1)
       GDF3     = DELAY(13,TDLYDF,GDF2)
       GDF      = GDF3*AKDF
*  CORRECTIVE ACTION ON TOP PRODUCT COMPOSITION
       GDM1     = REALPL(0.0,TAUDM1,VALVE)
       GDM2     = REALPL(0.0,TAUDM2,GDM1)
       GDM      = GDM2*AKDM
*  TOP PRODUCT COMPOSITION
       XD1      = GDF+GDM
       XD       = XD1*AKD
*  DEVIATION OF XD FROM SETPOINT
       ERRD = SETPT-XD
*  DISTURBANCE ON BOTTOM PRODUCT COMPOSITION
       GWF1     = REALPL(0.0,TAUWF1,FF)
       GWF2     = REALPL(0.0,TAUWF2,GWF1)
       GWF3     = DELAY(10,TDLYWF,GWF2)
       GWF      = GWF3*AKWF
*  CORRECTIVE ACTION ON BOTTOM PRODUCT COMPOSITION
       GWM1     = REALPL(0.0,TAUWM1,VALVE)
       GWM2     = REALPL(0.0,TAUWM2,GWM1)
       GWM3     = DELAY(12,TDLYWM,GWM2)
       GWM      = GWM3*AKWM
*  BOTTOM PRODUCT COMPOSITION
       XWC      = GWF+GWM
*  BOTTOM PRODUCT COMPOSITION MEASURED BY THE G. C.
       XW1      = DELAY(10,TDLYW,XWC)
       XW       = XW1*AKW
*  DEVIATION OF XW FROM SETPOINT
       ERRW     = SETPT-XWC
*  ERROR DETECTING CIRCUIT
       ERROR2   = ERROR*ERROR
       ERRD2    = ERRD*ERRD
       ERRW2    = ERRW*ERRW
       ERRES    = INTGRL(0.0,ERROR2)
       ERRD2S   = INTGRL(0.0,ERRD2)
       ERRW2S   = INTGRL(0.0,ERRW2)
```

```
*
*  TERMINAL SECTION OF THE MODEL
TERMINAL
TIMER    DELT=0.20, FINTIM=120.0, PRDEL=1.0, OUTDEL=1.0
PRINT    XD, VALVE, C8, XW, ERRES, ERRD2S, ERRW2S
PRTPLT   XD, XW, C8
LABEL              (R8-FB-FF-TAUI=10.0)
END
STOP
ENDJOB
```

```
*            CONTINUOUS SYSTEM MODELING PROGRAM
*            ----------------------------------
*
*
*       ******************************************
*       *                                        *
TITLE          CONTROL OF BOTTOM PRODUCT COMPOSITION
*       *                                        *
*       ******************************************
*
*
*  DESCRIPTIONS OF PARAMETERS
*       GDF       TRANSFER FUNCTION OF XD FOR LOAD CHANGES
*       GDM       TRANSFER FUNCTION OF XD FOR CHANGES IN
*                 THE MANIPULATIVE VARIABLE
*       GWF       TRANSFER FUNCTION OF XW FOR LOAD CHANGES
*       GWM       TRANSFER FUNCTION OF XW FOR CHANGES IN
*                 THE MANIPULATIVE VARIABLE
*       GR        TRANSFER FUNCTION FOR THE REBOILER
*       AKT       AKC*AKV*AKM
*       AKC       GAIN OF THE FEEDBACK CONTROLLER
*       AKV       GAIN OF THE CONTROL VALVE
*       AKM       GAIN OF THE SENSING ELEMENT
*       TAUI      INTEGRAL TIME (MIN.)
*       ERRES     I.S.E. OF BOTTOM PRODUCT COMPOSITION
*       ERRD2S    I.S.E. OF TOP PRODUCT COMPOSITION
*       XD        TOP PRODUCT COMPOSITION
*       XW        BOTTOM PRODUCT COMPOSITION
*       FF        LOAD CHANGES
*       SETPT     SET POINT
*
*  USAGE
*       IF FEEDBACK CONTROL ONLY IS DESIRED, SET AKFF = 0.0
*
*  REMARKS
*       SIMULATION USING DATA FROM THE U. OF A. DISTILLATION
*       COLUMN
*

*  DATA REQUIRED FOR THE SIMULATION
*  --------------------------------
*  DATA FOR THE TRANSFER FUNCTION  GDM
PARAMETER     AKDM = -24.802, TAUDM1 = 4.054, TAUDM2 = 16.031
PARAMETER     TDLYDM = 1.067
*  DATA FOR THE TRANSFER FUNCTION  GWM
PARAMETER     AKWM = -14.038, TAUWM1 = 2.120, TAUWM2 = 14.250
PARAMETER     TDLYWM = 3.326
*  DATA FOR THE TRANSFER FUNCTION  GDF
PARAMETER     AKDF =    6.455, TAUDF1 = 5.143, TAUDF2 = 18.243
PARAMETER     TDLYDF = 3.467
```

```
*  DATA FOR THE TRANSFER FUNCTION  GWF
PARAMETER      AKWF =   3.657, TAUWF1 = 0.628, TAUWF2 = 12.889
PARAMETER      TDLYWF = 3.649
*  DATA FOR THE TRANSFER FUNCTION GR
PARAMETER      AKR  = 1.000
*  DATA FOR THE CONTROL VALVE
PARAMETER      AKV  = 1.000
*  DATA FOR THE SENSING ELEMENT FOR TOP PRODUCT COMPOSITION
PARAMETER      AKD  = 1.000
*  DATA FOR THE SENSING ELEMENT OF BOTTOM COMPOSITION
PARAMETER      AKW = 1.000, TDLYW = 2.500
*  SETPOINT
CONSTANT       SETPT = 0.000
*  FORCING FUNCTION
PARAMETER      FF   = 0.430
*
*  FEEDBACK CONTROLLER CONSTANT
PARAMETER      AKT = 0.20
*  INTEGRAL TIME CONSTANT
PARAMETER      TAUI = 10.0
* ------------------------------


INITIAL
*  INITIALIZE PROCESS PARAMETERS
        AMEAS = 0.0

*


DYNAMIC
*  DYNAMIC SECTION OF THE MODEL
*  DEVIATION FROM SETPOINT
        ERROR = SETPT+AMEAS
*  PROPORTIONAL CONTROLLER CONSTANT
        AKC     = AKT/(AKV*AKM*AKR)
*  FEEDBACK CONTROLLER ( PROPORTIONAL PLUS INTEGRAL )
        CONT    = ERROR+INTGRL(0.0,ERROR/TAUI)
        CONTRL  = AKC*CONT
*  FEEDFORWARD CONTROLLER CONSTANT
        AKGP    = AKWM
        AKGL    = AKWF
        AKFF    = AKGL/(AKGP*AKV*AKR)
*  FEEDFORWARD COMPENSATION
        FEEDFD  = -FF*AKFF
*  SIGNAL TO THE VALVE
        SIGNAL  = CONTRL+FEEDFD
*  VALVE OUTPUT (STEAM FLOW RATE)
        REBLER  = SIGNAL*AKR
*  REBOIL VAPOR RATE
        VALVE   = AKV*REBLER
```

```
*  DISTURBANCE ON BOTTOM PRODUCT COMPOSITION
        GWF1     = REALPL(0.0,TAUWF1,FF)
        GWF2     = REALPL(0.0,TAUWF2,GWF1)
        GWF3     = DELAY(10,TDLYWF,GWF2)
        GWF      = GWF3*AKWF
*  CORRECTIVE ACTION ON BOTTOM PRODUCT COMPOSITION
        GWM1     = REALPL(0.0,TAUWM1,VALVE)
        GWM2     = REALPL(0.0,TAUWM2,GWM1)
        GWM3     = DELAY( 2,TDLYWM,GWM2)
        GWM      = GWM3*AKWM
*  BOTTOM PRODUCT COMPOSITION
        XW       = GWF+GWM
*  MEASUREMENT OF OUTPUT
        AMEA     = DELAY(10,TDLYW,XW)
        AMEAS    = AMEA*AKW
*  DISTURBANCE ON TOP PRODUCT COMPOSITION
        GDF1     = REALPL(0.0,TAUDF1,FF)
        GDF2     = REALPL(0.0,TAUDF2,GDF1)
        GDF3     = DELAY(13,TDLYDF,GDF2)
        GDF      = GDF3*AKDF
*  CORRECTIVE ACTION ON TOP PRODUCT COMPOSITION
        GDM1     = REALPL(0.0,TAUDM1,VALVE)
        GDM2     = REALPL(0.0,TAUDM2,GDM1)
        GDM3     = DELAY( 4,TDLYDM,GDM2)
        GDM      = GDM3*AKDM
*  TOP PRODUCT COMPOSITION
        XD1      = GDF+GDM
        XD       = XD1*AKD
*  DEVIATION OF XD FROM SETPOINT
        ERRD = SETPT-XD
*  ERROR DETECTING CIRCUIT
        ERROR2   = ERROR*ERROR
        ERRD2    = ERRD*ERRD
        ERRES    = INTGRL(0.0,ERROR2)
        ERRD2S   = INTGRL(0.0,ERRD2)
TIMER   DELT=0.20,FINTIM=120.0,PRDEL=1.0,OUTDEL=1.0
PRINT   XD, XW, ERRES, ERRD2S
LABEL          (SW-FB-FF-TAUI=10.0)
PRTPLT  XD, XW
END
STOP
ENDJOB
```

APPENDIX D

LISTINGS OF PROCESS PROGRAMS

The first part of this appendix contains all the necessary DDC control, data accumulation loops and ring buffers which have been employed during the experimental work. Exponential filters and thermocouple break filters have been used in all flow loops and temperature loops respectively to smooth the noisy data. A filter constant $\beta = 0.80$ has been associated with all the flow loops and a filter constant $\beta = 0.75$ has been used in all the temperature loops to attenuate the noise.

The second part of this appendix contains the listings of all process programs which have been used in this work, namely:

1. DASS
2. ONOFF
3. GTDAT

Associated subprograms and subroutines which have been written for each of these programs are included immediately following the main program. Also included in this appendix is a typical output of the process program DASS.

GAS CHROMATOGRAPH LOOP RECORDS

```
          ID = 0201     G. C. DATA ACQUISITION LOOP
01  4010  0004  004D  0000  BF00  7FFF  0000  0000  0000  0000
02  0000  0000  7FFF  0000  0000

          ID = 0202     G. C. DATA ACCUMULATION LOOP
01  067F  0000  0201  0000  0000  0000
```

DATA ACQUISITION LOOP RECORDS

A. CONTROL OF THE LIQUID TEMPERATURE ON AN INTERMEDIATE TRAY BY MANIPULATION OF REFLUX FLOW

```
            ID = 0170      FEED FLOW
01  621B  205C+04102  3340  8400+07214  0000  0000  0000  7FFF
02  7FFF  2990  7FFF  0000  2990  7FFF  0000  2990  106A  3FFB
03  0080  0000  0000  0000  0000  0000

            ID = 0171      REFLUX FLOW
01  6010  205F+04101  3340  8480+08364  0000  0000  0000  7FFF
02  7FFF  2110  7FFF  0000  2110

            ID = 0172      STEAM FLOW
01  6010  205F+04100  3340  8480+05740+00303  0000  0000  7FFF
02  7FFF  2110  7FFF  0000  2110

            ID = 0173      TOP PRODUCT FLOW
01  6010  205F+04103  3340  8480+05382  0000  0000  0000  7FFF
02  7FFF  2110  7FFF  0000  2110

            ID = 0174      BOTTOM PRODUCT FLOW
01  6010  205F+04104  3340  8480+05032  0000  0000  0000  7FFF
02  7FFF  2110  7FFF  0000  2110

            ID = 0175      TOP PRODUCT COMPOSITION
01  641E  404C+04105  0000  9100-01310+09879  0000  0000  7FFF
02  7FFF  2990  7FFF  0000  2910  7FFF  0000  2990  126A  0000
03  00C0  0000  0000  0000  0000  0000

            ID = 0176      TEMPERATURE OF TRAY 8
01  721E  10BC+00138  3000  A200+20000  0000  0000  0000  7FFF
02  7FFF  2990  7FFF  0000  2990  7FFF  0000  2990  116A  0000
03  0080  0000  0000  0000  0020  7000  0000  0000  0000

            ID = 0177      BOTTOM COMPOSITION (DUMMY)
01  4010  204F+20000  0000  9180+20000+00000  0000  0000  7FFF
02  7FFF  2110  7FFF  0000  2110
```

DATA ACQUISITION LOOP RECORDS ...(CONT'D)

```
                ID = 0178      BOTTOM COMPOSITION
01   0010   207F  0177  0000  9180+20000+00000  0000  0000  7FFF
02   7FFF   2110  7FFF  0000  2110
```

```
                ID = 0179      FEED COMPOSITION (DUMMY)
01   4010   204F+20000  0000  9180+20000  0000  0000  0000  7FFF
02   7FFF   2110+10000  0000  2110
```

```
                ID = 0180      FEED COMPOSITION
01   0010   207F  0179  0000  9180+20000  0000  0000  0000  7FFF
02   7FFF   2110+10000  0000  2110
```

B. CONTROL OF THE LIQUID TEMPERATURE ON AN INTERMEDIATE TRAY BY MANIPULATION OF STEAM FLOW

ALL THE DDC LOOPS REMAIN THE SAME AS WITH REFLUX CONTROL EXCEPT THE 2 FOLLOWING LOOP RECORDS

```
                ID = 0175      TOP PRODUCT COMPOSITION
01   641E   404C+04105  0000  9100-01310+09879  0000  0000  7FFF
02   7FFF   2990  7FFF  0000  2990  7FFF  0000  2990  116A  23D4
03   00C0   0000  0000  0000  001B  0C00  0000  0000  0400
```

```
                ID = 0176      TEMPERATURE OF TRAY 1
01   721E   10BC+00131  3000  A200+20000  0000  0000  0000  7FFF
02   7FFF   2990  7FFF  0000  2990  7FFF  0000  2990  126A  2663
03   00C0   0000  0000  0000  0801  0301  0000  0000  0000
```

N. B. CONTROL OF THE LIQUID TEMPERATURE OF ANY INTERMEDIATE TRAY CAN BE PERFORMED BY MODIFYING THE MULTIPLEX ADDRESS IN THE TEMPERATURE LOOP RECORD

DATA ACQUISITION LOOPS FOR INTERMEDIATE TRAY TEMPERATURES

```
              ID = 0181      TEMPERATURE OF TRAY 1
01   7010   21BF+00131  0000  A280+20000  0000  0000  0000  7FFF
02   7FFF   2110  7FFF  0000  2110

              ID = 0182      TEMPERATURE OF TRAY 2
01   7010   21BF+00132  0000  A280+20000  0000  0000  0000  7FFF
02   7FFF   2110  7FFF  0000  2110

              ID = 0183      TEMPERATURE OF TRAY 3
01   7010   21BF+00133  0000  A280+20000  0000  0000  0000  7FFF
02   7FFF   2110  7FFF  0000  2110

              ID = 0184      TEMPERATURE OF TRAY 4
01   7010   21BF+00134  0000  A280+20000  0000  0000  0000  7FFF
02   7FFF   2110  7FFF  0000  2110

              ID = 0185      TEMPERATURE OF TRAY 5
01   7010   21BF+00135  0000  A280+20000  0000  0000  0000  7FFF
02   7FFF   2110  7FFF  0000  2110

              ID = 0186      TEMPERATURE OF TRAY 6
01   7010   21BF+00136  0000  A280+20000  0000  0000  0000  7FFF
02   7FFF   2110  7FFF  0000  2110

              ID = 0187      TEMPERATURE OF TRAY 7
01   7010   21BF+00137  0000  A280+20000  0000  0000  0000  7FFF
02   7FFF   2110  7FFF  0000  2110

              ID = 0188      TEMPERATURE OF TRAY 8
01   7010   21BF+00138  0000  A280+20000  0000  0000  0000  7FFF
02   7FFF   2110  7FFF  0000  2110
```

RING BUFFERS FOR CONTROL STUDY

```
          ID = 0210      FEED FLOW
01  060E  5408  0170  0000  0000  0200

          ID = 0211      REFLUX FLOW
01  060E  5408  0171  0000  0000  0200

          ID = 0212      STEAM FLOW
01  060E  5408  0172  0000  0000  0200

          ID = 0213      TOP PRODUCT FLOW
01  060E  5408  0173  0000  0000  0200

          ID = 0214      BOTTOM PRODUCT FLOW
01  060E  5408  0174  0000  0000  0200

          ID = 0215      TOP PRODUCT COMPOSITION
01  060E  5408  0175  0000  0000  0200

          ID = 0216      BOTTOM COMPOSITION
01  060E  5408  0178  0000  0000  0200

          ID = 0217      FEED COMPOSITION
01  060E  5408  0180  0000  0000  0200

          ID = 0221      TEMPERATURE OF TRAY 1
01  060E  5408  0181  0000  0000  0200

          ID = 0222      TEMPERATURE OF TRAY 2
01  060E  5408  0182  0000  0000  0200

          ID = 0223      TEMPERATURE OF TRAY 3
01  060E  5408  0183  0000  0000  0200
```

RING BUFFERS FOR CONTROL STUDY ...(CONT'D)

```
          ID = 0224      TEMPERATURE OF TRAY 4
01  060E  5408  0184  0000  0000  0200

          ID = 0225      TEMPERATURE OF TRAY 5
01  060E  5408  0185  0000  0000  0200

          ID = 0226      TEMPERATURE OF TRAY 6
01  060E  5408  0186  0000  0000  0200

          ID = 0227      TEMPERATURE OF TRAY 7
01  060E  5408  0187  0000  0000  0200

          ID = 0228      TEMPERATURE OF TRAY 8
01  060E  5408  0188  0000  0000  0200
```

MAINLINE DASS

```
      MAINLINE DASS
C
C
C          ************************************
C          *                                  *
C          *          PROGRAM   DASS          *
C          *          ---------------         *
C          *                                  *
C          ************************************
C
C
C     PURPOSE
C        START DATA ACQUISITION FOR STEADY-STATE DATA AND
C        PERFORM MATERIAL AND ENERGY BALANCES CALCULATIONS
C
C     DESCRIPTION OF PARAMETERS
C        MAX       NUMBER OF SAMPLED DATA POINTS
C        TIME      SAMPLE TIME (SEC.)
C        RUN       RUN NUMBER
C        DATE      DATE OF THE EXPERIMENT
C        BTCMP     BOTTOM PRODUCT COMPOSITION
C        FDCMP     FEED COMPOSITION
C        FDPLT     FEED TRAY
C
C     USAGE
C        QUEUE FROM TELETYPE 8 AND ENTER DATA AS REQUIRED
C        EXAMPLE
C        ENTER--MAX, TIME, RUN(2A4), DATE(2A4)
C        $10 10 FB-RI805, JAN 01
C        ENTER BOTTOM COMPOSITION,FEED COMPOSITION AND FEED
C        $0.6 47.0 4
C        DATAC QUEUED
C
C     REMARKS
C        DASS IS A PROCESS PROGRAM OPERATED IN VCORE UNDER
C        MPX
C
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C        DATAC
C
C

      INTEGER FDPLT
      EXTERNAL DATAC
      DIMENSION RUN(2), DATE(2), TITLE(10,3)
      DIMENSION ZERO(32)
      DATA ZERO/32*0./
      DEFINE FILE 10(60,80,U,NEXT)
      KOUNT=0
```

MAINLINE DASS ...(CONT'D)

```
      LUR = 8
      LUW = LUR
      WRITE (LUW,5)
    5 FORMAT (T5, 'ENTER OPTION-1=GO, 2=STOP')
    6 CALL FFINP(LUR,1,10,IOPT,IER)
      IF (IER) 6,7,6
    7 GO TO (9,90), IOPT
    9 WRITE (LUW,10)
   10 FORMAT (T5, 'ENTER--MAX, TIME, RUN(2A4), DATE(2A4)')
   15 CALL FFINP(LUR,4,10,MAX,10,IPOL,23,RUN,23,DATE,IER)
      IF (IER) 20,40,30
   20 WRITE (LUW,25)
   25 FORMAT (T5, 'CALL TO FFINP IN ERROR--CRASH')
      CALL EXIT
   30 WRITE (LUW,35)
   35 FORMAT (T5, 'INPUT  TO FFINP IN ERROR-TRY AGAIN')
      GO TO 15
   40 CONTINUE
      WRITE(LUW,41)
   41 FORMAT (T5, 'ENTER BOTTOM COMPOSITION,FEED COMPOSITION
     * AND FEED ')
   42 CALL FFINP(LUR,3,1,BTCMP,1,FDCMP,0,FDPLT,IER)
      IF(IER)20,43,42
   43 READ (10'1) NLOOP
      WRITE (10'1) NLOOP,KOUNT,MAX,IPOL,BTCMP,FDCMP,FDPLT
      READ (10'4) ((TITLE(I,J), J=1,3), I=1,10)
      WRITE (10'4) ((TITLE(I,J), J=1,3), I= 1,10), (RUN(I),
     * I=1,2),
     1  (DATE(I), I=1,2)
      WRITE(10'8)(ZERO(I),I=1,32)
      WRITE(10'9)(ZERO(I),I=1,32)
      IT = 9
      CALL QLEVL(DATAC,1,0,0,IEQ)
      GO TO (170,172,174),IEQ
  170 CONTINUE
      WRITE (LUW,70)
   70 FORMAT (T5, 'DATAC QUEUED')
      CALL EXIT
  172 CONTINUE
      WRITE (LUW,72)
   72 FORMAT (T5, 'QUEUE TABLE IS FULL')
      CALL EXIT
  174 CONTINUE
      WRITE (LUW,74)
   74 FORMAT (T5, 'PROGRAM WAS QUEUED')
      CALL EXIT
   90 IT = 9
      CALL CANCL(IT)
      CALL EXIT
      END
```

SUBPROGRAM DATAC

```
      SUBPROGRAM DATAC
C
C
C                    SUBPROGRAM  DATAC
C                    -----------------
C
C
C     PURPOSE
C        DATA ACQUISITION FOR MATERIAL AND ENERGY BALANCES
C        CALCULATIONS
C
C     USAGE
C        THIS SUBPROGRAM IS QUEUED BY DASS AT EVERY SAMPLED
C        INTERVAL FOR MATERIAL AND ENERGY BALANCES
C        CALCULATIONS
C
C     REMARKS
C        USE OF THIS SUBPROGRAM WOULD SUSPEND EXECUTION OF
C        OTHER PROGRAMS IN VCORE FOR A PERIOD WHICH WAS SPE-
C        CIFIED BY THE USER IN THE PROCESS PROGRAM DASS
C
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C        DASS, BALNC
C
C

      EXTERNAL BALNC
      EXTERNAL DATAC
      DIMENSION A(32),B(32),TOT(32),SUMSQ(32),ICODE(32)
      DEFINE FILE 10(60,80,U,INXT)

C     MULTIPLEXOR NUMBER AND CALCULATION CODE

      DATA ICODE/14102,14101,14100,14104,14103,14105,24106
     *,24109,24107,
     124108,24110,30130,30131,30132,30133,30134,30135,30136
     *,30137,30138,
     230139,30140,30141,30142,30143,30144,30145,30146,30147
     *,30148,
     330149,30150/

C     SPAN/32767

      DATA A/1.1008E-04,1.2762E-04,.8758E-04,.7678E-04
     *,.8212E-04,
     121.0333E-04,-2.0100E-04,.6103E-03,3.6622E-04,3.6622E
     *-04,
     23.6622E-04,21*0./
```

SUBPROGRAM DATAC ...(CONT'D)

```
C       INTERCEPT

        DATA B/2*0.,0.3,3*0.,98.79,-10.,3*3.,21*0./

        READ (10'1) NLOOP, KOUNT, MAX ,IPOL
        READ(10'8)(TOT(I),I=1,32)
        READ(10'9)(SUMSQ(I),I=1,32)
        DO 999 KOUNT = 1,MAX

C       CALCULATE COLD JUNCTION COMPENSATION

        CALL COLDJ(IRBT)
        DO 140 I=1,32

C       GET CALCULATION TYPE

        ITYPE=ICODE(I)/10000

C       CALCULATE MPX ADDRESS

        MPXAD=ICODE(I)-10000*ITYPE

C       READ MULTIPLEXOR

        CALL AIP(11000,INPUT,MPXAD)
20      CALL AIP(0,JTEST)
        GO TO(20,40),JTEST
40      DATA=INPUT
        GO TO(60,80,100),ITYPE

C       FLOW CALCULATION

60      CALL ZERCK(DATA)

C       TAKE SQUARE ROOT AND RESCALE INPUT

        DATA=SQRT(DATA)*181.0166
        GO TO 110

C       ZERO CHECK ONLY

80      CALL ZERCK(DATA)
        GO TO 110

C       TEMPERATURE CALCULATION

100     CALL TCONV(DATA,INPUT,IRBT)
        GO TO 120
110     DATA=A(I)*DATA+B(I)
120     TOT(I)=TOT(I)+DATA
```

SUBPROGRAM DATAC ...(CONT'D)

```
      SUMSQ(I)=SUMSQ(I)+DATA*DATA
140   CONTINUE
      WRITE (10'1) NLOOP, KOUNT, MAX
      WRITE(10'8)(TOT(I),I=1,32)
      WRITE(10'9)(SUMSQ(I),I=1,32)

C     CHECK IF ENOUGH POINTS ACCUMULATED

      TIME=IPOL
      INT=TIME/0.1
      CALL SUSPN (9,INT)
  999 CONTINUE
      CALL QLEVL(BALNC,1,0,0,IER)
      CALL DEQUE(DATAC,1,0)
      CALL CANCL(9)
      CALL EXIT
      END
```

SUBPROGRAM BALNC

```
      SUBPROGRAM BALNC
C
C
C                     SUBPROGRAM  BALNC
C                     -----------------
C
C
C     PURPOSE
C        PERFORM MATERIAL AND ENERGY BALANCES CALCULATIONS
C        WHEN DATA ACCUMULATION HAS BEEN COMPLETED
C
C     USAGE
C        THIS PROGRAM IS QUEUED BY DATAC TO OBTAIN NECESSARY
C        DATA
C
C     REMARKS
C        THIS IS A PROCESS PROGRAM OPERATED IN VCORE UNDER
C        MPX
C
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C        COLDJ, TCONV, ZERCK, INFF
C
C

      INTEGER FDPLT
      DIMENSION RUN(2), DATE(2)
      DIMENSION AV(34),VAR(34),TITLE(34,3), UNIT(34,2)
      DEFINE FILE 10(60,80,U,NEXT)

C     DEFINE FUNCTION STATEMENTS

      TEMP(T)=5.*(T-32.)/9.
      CPWG(T)=7.880+0.32E-02*T-483.3E-05*T**2
      CPWL(T)=1.0009-0.1362E-03*T+0.2026E-05*T**2
      CPMG(T)=10.26+1.984E-02*T-0.144E-05*T**2-1.92E-09*T**3
      CPML(T)=0.5573+0.1870E-02*T+0.9011E-05*T**2
      HEATW(T)=1080.2-0.3785*T-0.5618E-03*T**2
      HEATM(T)=(291.2-0.3308*T-0.1526E-02*T**2)*1.8
      DENS(T,X)=1.0201-0.5123E-03*T-0.1512E-05*T**2-0.1519E
     *-02*100.*X
     1   -0.8106E-05*(100.*X)**2
      DENSW(T)=1.0050-0.2142E-03*T-0.2508E-05*T**2

C      READ DATA
C

      READ (10'1) NLOOP,KOUNT,MAX,IPOL,BTCMP,FDCMP,FDPLT
      READ (10'2) ((TITLE(I,J), J=1,3), I=1,12)
      READ (10'3)  ((TITLE(I,J), J=1,3), I=13,24)
```

SUBPROGRAM BALNC ...(CONT'D)

```
      READ (10'4) ((TITLE(I,J), J=1,3), I=25,34), (RUN(I),
     * I=1,2),
     1  (DATE(I), I=1,2)
      READ (10'5) ((UNIT(I,J), J=1,2), I=1,18)
      READ (10'6) ((UNIT(I,J), J=1,2), I=19,34)
      READ(10'8)(AV(I),I=1,32)
      READ(10'9)(VAR(I),I=1,32)
C     COMPUTE AVERAGE AND VARIANCE OF READINGS
C
      DO 1 I=1,32
      VAR(I)=(VAR(I)-AV(I)*AV(I)/KOUNT)/(KOUNT-1)
      VAR(I)=SQRT(VAR(I))
1     AV(I)=AV(I)/KOUNT
C
C     INSERT FEED AND BOTTOM COMPOSITIONS IN VECTOR
C
      DO 2 I=1,32
      K=35-I
      IF(K-10)4,3,3
3     AV(K)=AV(K-2)
      VAR(K)=VAR(K-2)
2     CONTINUE
4     VAR(8)=0.
      VAR(9)=0.
      AV(8)=BTCMP
       AV(9)=FDCMP
C      CORRECT FLOW SIGNALS FOR TEMPERATURE
C
      F=AV(1)*SQRT(DENS(TEMP(AV(27)),AV(9)/100.))
      R=AV(2)*SQRT(DENS(TEMP(AV(26)),AV(7)/100.))
      B=AV(4)*SQRT(DENS(TEMP(AV(28)), AV(8)/100.))
      D=AV(5)*SQRT(DENS(TEMP(AV(26)),AV(7)/100.))
      W=AV(6)*SQRT(DENSW(TEMP(AV(33))))
C        OVERALL MATERIAL BALANCE
C
      FIN=F
      FOUT=D+B
      ERRT=(FOUT/FIN-1.)*100.
C      COMPONENT BALANCE
      CIN1=F*AV(9)/100.
```

SUBPROGRAM BALNC ...(CONT'D)

```
      CIN2=F*(1.-AV(9)/100.)
      CT1=D*AV(7)/100.
      CT2=D*(1.-AV(7)/100.)
      CB1=B*AV(8)/100.
      CB2=B*(1.-AV(8)/100.)
      COUT1=CT1+CB1
      COUT2=CT2+CB2
      ERR1=(COUT1/CIN1-1.)*100.
      ERR2=(COUT2/CIN2-1.)*100.
C        OVERALL ENERGY BALANCE
C
C        ENTHALPY BASED ON ZERO DEG F
C
C       FEED ENTHALPY IN
      HFI1=CPML(TEMP(AV(30)))*AV(9)/100.*F*AV(30)
      HFI2=CPWL(TEMP(AV(30)))*(1.-AV(9)/100.)*F*AV(30)
      HFI=HFI1+HFI2
C       STEAM ENTHALPY IN
      HSI=(HEATW(AV(24))+CPWL(TEMP(AV(24)))*AV(24))*AV(3)
C       REFLUX ENTHALPY IN
      HRI1=CPML(TEMP(AV(31)))*R*AV(7)/100.*AV(31)
      HRI2=CPWL(TEMP(AV(31)))*R*(1.-AV(7)/100.)*AV(31)
      HRI=HRI1+HRI2
C       COOLING WATER ENTHALPY IN
      HWI=CPWL(TEMP(AV(33)))*W*AV(33)
C       TOTAL ENTHALPY IN
      HIT=HFI+HSI+HRI+HWI
C       BOTTOM ENTHALPY OUT
      HBO1=CPML(TEMP(AV(14)))*B*AV(8)/100.*AV(14)
      HBO2=CPWL(TEMP(AV(14)))*B*(1.-AV(8)/100.)*AV(14)
      HBO=HBO1+HBO2
C       TOP PRODUCT ENTHALPY OUT
      HTO1=CPML(TEMP(AV(23)))*D*AV(7)/100.*AV(23)
      HTO2=CPWL(TEMP(AV(23)))*D*(1.-AV(7)/100.)*AV(23)
      HTO=HTO1+HTO2
```

SUBPROGRAM BALNC ...(CONT'D)

```
C        REFLUX ENTHALPY OUT

       HRO1=CPML(TEMP(AV(23)))*R*AV(7)/100.*AV(23)
       HRO2=CPWL(TEMP(AV(23)))*R*(1.-AV(7)/100.)*AV(23)
       HRO=HRO1+HRO2

C        STEAM CONDENSATE ENTHALPY OUT

       HSO=CPWL(TEMP(AV(25)))*AV(3)*AV(25)

C        COOLING WATER ENTHALPY OUT

       HWO=CPWL(TEMP(AV(34)))*W*AV(34)

C        TOTAL ENTHALPY OUT

       HOT=HBO+HTO+HRO+HSO+HWO

C        DIFFERENCE IS HEAT LOSS

       HLOSS=HIT-HOT

C      DOCUMENT STEADY STATE, MATERIAL AND ENERGY BALANCES
C
C      STEADY STATE
C

       WRITE (6,5)
     5 FORMAT ('1',//////)
       WRITE (6,6) (RUN(I), I=1,2), (DATE(I), I=1,2)
     6 FORMAT (T51, 'STEADY STATE DATA'/T52, 'RUN NO ', 2A4
      */T55, 2A4//)
       WRITE (6,900) (TITLE(1,J), J=1,3), F, (UNIT(1,J), J=1
      *,2),
      1              (TITLE(4,J), J=1,3), B, (UNIT(4,J), J=1
      *,2)
   900 FORMAT (T32, 3A4, T47, F6.3, 2A4, T62, 3A4, T77, F6.3,
      * 2A4)
       WRITE (6,900) (TITLE(2,J), J=1,3), R, (UNIT(2,J), J=1
      *,2),
      1              (TITLE(5,J), J=1,3), D, (UNIT(5,J), J=1
      *,2)
       WRITE (6,900) (TITLE(3,J), J=1,3), AV(3),  (UNIT(3,J),
      * J=1,2),
      1              (TITLE(6,J), J=1,3), W, (UNIT(6,J), J=1
      *,2)
       WRITE (6,901) FDPLT, (TITLE(9,J), J=1,3), FDCMP,
      * (UNIT(9,J),J=1,2)
   901 FORMAT (T32, 'FEED PLATE', T47, I3, T62, 3A4, T77,
      * F6.2, 2A4)
```

```
      WRITE (6,902) (TITLE(7,J), J=1,3), AV(7), (UNIT(7,J),
     * J=1,2),
     1              (TITLE(8,J), J=1,3), AV(8), (UNIT(8,J),
     * J=1,2)
  902 FORMAT (T32, 3A4, T47, F6.2, 2A4, T62, 3A4, T77, F6.2,
     * 2A4)
      WRITE (6,903) (TITLE(30,J), J=1,3), AV(30), (UNIT(30
     *,J), J=1,2),
     1              (TITLE(31,J), J=1,3), AV(31), (UNIT(31
     *,J), J=1,2)
  903 FORMAT (T32, 3A4, T47, F6.1, 2A4, T62, 3A4, T77, F6.1,
     * 2A4)
      WRITE (6,903) (TITLE(24,J), J=1,3), AV(24), (UNIT(24
     *,J), J=1,2),
     1              (TITLE(10,J), J=1,3), AV(10), (UNIT(10
     *,J), J=1,2)
      WRITE (6,60)
C       MATERIAL BALANCE
C
      WRITE (6,10)
   10 FORMAT (T44, 'M A T E R I A L   B A L A N C E'//T56,
     * 'FLOW', T66,
     1 'COMP', T73, 'METHANOL', T84, 'WATER',/T54, '(LB
     */MIN)', T64,
     2 '(WT PCT)', T73, '(LB/MIN)', T83,  '(LB/MIN)')
      WRITE (6,20) F, AV(9), CIN1, CIN2
   20 FORMAT (/T32, 'FEED', T54, F6.3, T64, F6.3, T73, F6.3,
     * T83, F6.3)
      WRITE (6,30) B, AV(8), CB1, CB2
   30 FORMAT (T32, 'BOTTOM PRODUCT', T54, F6.3, T64, F6.3,
     * T73, F6.3,
     1   T83, F6.3)
      WRITE (6,40) D, AV(7), CT1, CT2
   40 FORMAT (T32, 'TOP PRODUCT', T54, F6.3, T64, F6.3, T73,
     * F6.3, T83,
     1   F6.3)
      WRITE (6,50) ERRT, ERR1, ERR2
   50 FORMAT (T32, 'CLOSURE ERROR-PC', T53, F5.1, T72, F5.1,
     * T82, F5.1)
      WRITE (6,60)
   60 FORMAT (////)
C       ENERGY BALANCE
C
      WRITE (6,70)
   70 FORMAT (T47, 'E N E R G Y   B A L A N C E'//T57,
     * 'ENTHALPY IN',
```

SUBPROGRAM BALNC ...(CONT'D)

```
    1  T74, 'ENTHALPY OUT'/T58, '(BTU/MIN)', T75, '(BTU
   */MIN)')
      WRITE (6,80) HWI, HWO
   80 FORMAT (/T39, 'COOLING WATER', T58, F7.1, T76, F7.1)
      WRITE (6,90) HRI, HRO
   90 FORMAT (T39, 'REFLUX', T58, F7.1, T76, F7.1)
      WRITE (6,100) HTO
  100 FORMAT (T39, 'TOP PRODUCT', T76, F7.1)
      WRITE (6,110) HFI
  110 FORMAT (T39, 'FEED', T58, F7.1)
      WRITE (6,120) HSI, HSO
  120 FORMAT (T39, 'STEAM', T58, F7.1, T76, F7.1)
      WRITE (6,130) HBO
  130 FORMAT (T39, 'BOTTOM PRODUCT', T76, F7.1)
      WRITE (6,140) HIT, HOT
  140 FORMAT (T39, 'TOTAL', T58, F7.1, T76, F7.1)
      WRITE (6,150) HLOSS
  150 FORMAT (T39, 'HEAT LOSS', T76, F7.1)

C       DOCUMENT ALL STEADY STATE CONDITIONS
C

      WRITE (6,200)
  200 FORMAT ('1', //////)
      WRITE (6,210) KOUNT, (RUN(I), I=1,2), (DATE(I), I=1,2)
  210 FORMAT (T33, 'STEADY STATE CONDITIONS BASED ON', I4, '
   * POINTS'/
    1          T42, 'RUN NO ', 2A4, 1X, 2A4/)
      DO 230 I=1,13
      WRITE (6,220) (TITLE(I,J), J=1,3),AV(I),(UNIT(I,J),
   * J=1,2),VAR(I)
  220 FORMAT (T33, 3A4, '=', F7.3, 1X, 2A4, 3X, 'DEV=',
   * F7.4)
  230 CONTINUE
      DO 250 I=14,34
      WRITE (6,240)  (TITLE(I,J), J=1,3),AV(I),(UNIT(I,J),
   * J=1,2),VAR(I)
  240 FORMAT (T33, 3A4, '=', F7.1, 1X, 2A4, 3X, 'DEV=',
   * F7.4)
  250 CONTINUE
      WRITE (6,260)
  260 FORMAT ('1')
      CALL EXIT
      END
```

SUBROUTINE COLDJ

```
      SUBROUTINE COLDJ(IRBT)
C
C
C                    SUBROUTINE  COLDJ
C                    -----------------
C
C
C     PURPOSE
C        CALCULATE COLD JUNCTION COMPENSATION FOR TEMPERA-
C        TURE
C
C     DESCRIPTION OF PARAMETERS
C        IRBT     COLD JUNCTION COMPENSATION
C
C     USAGE
C        CALL COLDJ(RBT)
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C        NONE
C
C
      DIMENSION MPXAD(2),INPUT(2)
      DATA C,D/94.429,-3082.0428/
      DATA MPXAD/129,128/
C     129 = BRIDGE UNBALANCE,  128 = REF VOLTAGE
      DO 40 I=1,2
      CALL AIP(11000,INPUT(I),MPXAD(I))
   20 CALL AIP(0,JTEST)
      GO TO(20,40),JTEST
   40 CONTINUE
      TRBT=51.876*FLOAT(INPUT(1))/FLOAT(INPUT(2))+41.0
      IRBT=C*TRBT+D
      RETURN
      END
```

SUBROUTINE TCONV

```
      SUBROUTINE TCONV(TEMP,INPUT,IRBT)
C
C                    SUBROUTINE  TCONV
C                    -----------------
C
C
C     PURPOSE
C        CALCULATE THE TEMPERATURE FROM THE MULTIPLEXOR
C        READING AND THE COLD JUNCTION COMPENSATION
C
C     DESCRIPTION OF PARAMETERS
C        TEMP      COMPENSATED TEMPERATURE IN DEG F
C        INPUT     MULTIPLEXOR READIND IN BINARY COUNTS
C        IRBT      COLD JUNCTION COMPENSATION
C
C     USAGE
C        CALL TCONV(TEMP,INPUT,RBT)
C
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C        NONE
C
C

      INTEGER COUNT(9)
      REAL INTCP(9)
      DIMENSION SLOPE(9)
      DATA COUNT/1639,3998,6357,8749,11174,13631,16089,18546
     *,21036/
      DATA SLOPE/.01059,.01059,.01045,.01031,.01017,.01017
     *,.01017,
     1.01003,.01003/
      DATA INTCP/32.6389,32.6389,33.5616,34.7974,36.3332
     *,36.3334,36.3333
     1,38.8156,38.8159/

C     COLD JUNCTION COMPENSATION

      INPUT=INPUT+IRBT

C     SEARCH FOR SEGMENT

      DO 20 I=1,9
      IF(COUNT(I)-INPUT)20,20,40
   40 INDX=I-1
      GO TO 60
   20 CONTINUE
   60 TEMP=SLOPE(INDX)*INPUT+INTCP(INDX)
      RETURN
      END
```

SUBROUTINE ZERCK

```
      SUBROUTINE ZERCK(INPUT)
C
C
C                      SUBROUTINE  ZERCK
C                      -----------------
C
C
C     PURPOSE
C        ZERO CHECK
C
C     DESCRIPTION OF PARAMETERS
C        INPUT    MULTIPLEXOR READING IN BINARY COUNTS
C
C     USAGE
C        CALL ZERCK(INPUT)
C
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C        NONE
C
C

      REAL INPUT
      INPUT=INPUT-6553.4

C     ZERO CHECK INPUT

      IF(INPUT)20,20,40
   20 INPUT=0.
      GO TO 60

C     RESCALE INPUT

   40 INPUT=INPUT*1.25
   60 RETURN
      END
```

PROGRAM INFF

```
      PROGRAM INFF

C
C
C                     PROGRAM  INFF
C                     -------------
C
C
C     PURPOSE
C        READ INTO DISK STORAGE FILE 'PAC01' THE TITLES
C        WHICH WILL BE USED FOR PROGRAM BALNC OUTPUT
C
C     DESCRIPTION OF PARAMETERS
C        TITLE    TITLES FOR SUBPROGRAM OUTPUT
C        UNIT     UNITS OF THE CORRESPONDING TITLES
C
C     USAGE
C        STORE THIS NONPROCESS PROGRAM ONTO DISK - THE
C        FOLLOWING DATA ARE REQUIRED FOR THIS PROGRAM INFF
C             FEED FLOW    LB/MIN
C             REFLUX FLOW  LB/MIN
C             STEAM FLOW   LB/MIN
C             BOTTOM PROD  LB/MIN
C             TOP PROD     LB/MIN
C             COOL WATER   LB/MIN
C             TOP PROD     WT P C
C             BOTTOMS COMP WT P C
C             FEED COMP    WT P C
C             PRESSURE     IN H2O
C             COND LEVEL   PSIG
C             REB'R LEVEL  PSIG
C             DIFF PRESS   PSIG
C             REBOILER TEM DEG F
C             PLATE 1 TEMP DEG F
C             PLATE 2 TEMP DEG F
C             PLATE 3 TEMP DEG F
C             PLATE 4 TEMP DEG F
C             PLATE 5 TEMP DEG F
C             PLATE 6 TEMP DEG F
C             PLATE 7 TEMP DEG F
C             PLATE 8 TEMP DEG F
C             COND TEMP    DEG F
C             STEAM TEMP   DEG F
C             COND'T TEMP  DEG F
C             REFLUX FLOW  DEG F
C             FEED FLOW    DEG F
C             BOTTOM FLOW  DEG F
C             REB O'HEAD   DEG F
C             FEED INLET   DEG F
C             REFLUX INLET DEG F
```

PROGRAM INFF ...(CONT'D)

```
C                COL O'HEAD    DEG F
C                WATER INLET   DEG F
C                WATER OUTLET  DEG F
C           (ALL THESE DATA SHOULD START AT COLUMN 1 ON THE
C           DATA CARDS)
C
C        REMARKS
C           DATA FILE 10 OF NAME PAC01 IS REQUIRED
C
C

         DIMENSION TITLE(34,3), LPID(34), LPHX(34), UNIT(34,2)
         DATA NLOOP/34/
         DATA LPID/0120,0121,0122,0123,0124,0125,0126,0127,0128
        *,0129,0130,
        1            0131,0132,0135,0136,0137,0138,0139,0140,0141
        *,0142,0143,
        2            0144,0145,0146,0147,0148,0149,0150,0151,0152
        *,0153,0154,
        3            0155/
         DEFINE FILE 10(60,80,U,NEXT)
         DO 20 I=1,34
         READ (5,10) (TITLE(I,J), J=1,3), (UNIT(I,J), J=1,2)
         WRITE (6,15) (TITLE(I,J), J=1,3), (UNIT(I,J), J=1,2)
      10 FORMAT (5A4)
      15 FORMAT (T5, 5A4)
      20 CONTINUE
         DO 40 I=1,34
         LPID(I)=LPID(I)+100
         CALL CVID(LPID(I),LPHX(I))
40       CONTINUE
         KOUNT=0
         MAX=0
         A=0
         WRITE (10'1) NLOOP, KOUNT, MAX, A, A, KOUNT, (LPID(I),
        * I=1,NLOOP),
        1   (LPHX(I), I=1,NLOOP)
         WRITE (10'2) ((TITLE(I,J), J=1,3), I=1,12)
         WRITE (10'3) ((TITLE (I,J), J=1,3), I=13,24)
         WRITE (10'4) ((TITLE (I,J), J=1,3), I=25,34)
         WRITE (10'5) ((UNIT(I,J), J=1,2), I=1,18)
         WRITE (10'6) ((UNIT(I,J), J=1,2), I=19,34)
         CALL EXIT
         END
```

TABLE D.2-1

TYPICAL OUTPUT OF PROCESS PROGRAM DASS
(MATERIAL AND ENERGY BALANCES CALCULATIONS)

STEADY STATE DATA
RUN NO FB-I802
OCT 03

FEED FLOW	2.466 LB/MIN	BOTTOM PROD	1.252 LB/MIN
REFLUX FLOW	1.990 LB/MIN	TOP PROD	1.236 LB/MIN
STEAM FLOW	1.997 LB/MIN	COOL WATER	62.266 LB/MIN
FEED PLATE	4	FEED COMP	47.00 WT P C
TOP PROD	95.79 WT P C	BOTTOMS COMP	0.70 WT P C
FEED INLET	163.5 DEG F	REFLUX INLET	150.6 DEG F
STEAM TEMP	233.1 DEG F	PRESSURE	1.1 IN H2O

M A T E R I A L   B A L A N C E

	FLOW (LB/MIN)	COMP (WT PCT)	METHANOL (LB/MIN)	WATER (LB/MIN)
FEED	2.466	47.000	1.159	1.307
BOTTOM PRODUCT	1.252	0.700	0.008	1.244
TOP PRODUCT	1.236	95.790	1.184	0.052
CLOSURE ERROR-PC	0.9		2.8	-0.8

E N E R G Y   B A L A N C E

	ENTHALPY IN (BTU/MIN)	ENTHALPY OUT (BTU/MIN)
COOLING WATER	3736.5	5302.5
REFLUX	219.3	206.6
TOP PRODUCT		128.3
FEED	354.9	
STEAM	2390.7	464.1
BOTTOM PRODUCT		264.6
TOTAL	6701.5	6366.2
HEAT LOSS		335.2

TABLE D.2-1 ...(CONT'D)

TYPICAL OUTPUT OF PROCESS PROGRAM DASS
(STEADY STATE OPERATING CONDITIONS)

STEADY STATE CONDITIONS BASED ON 10 POINTS
RUN NO FB-I802 OCT 03

FEED FLOW =	2.580	LB/MIN	DEV= 0.0049
REFLUX FLOW =	2.268	LB/MIN	DEV= 0.0227
STEAM FLOW =	1.997	LB/MIN	DEV= 0.0059
BOTTOM PROD =	1.254	LB/MIN	DEV= 0.0045
TOP PROD =	1.409	LB/MIN	DEV= 0.0119
COOL WATER =	62.233	LB/MIN	DEV= 0.4381
TOP PROD =	95.790	WT P C	DEV= 0.0373
BOTTOMS COMP=	0.700	WT P C	DEV= 0.0000
FEED COMP =	47.000	WT P C	DEV= 0.0000
PRESSURE =	1.123	IN H2O	DEV= 0.0039
COND LEVEL =	5.004	PSIG	DEV= 0.0158
REB'R LEVEL =	9.903	PSIG	DEV= 0.0594
DIFF PRESS =	9.978	PSIG	DEV= 0.1103
REBOILER TEM=	209.9	DEG F	DEV= 0.4625
PLATE 1 TEMP=	204.3	DEG F	DEV= 0.2713
PLATE 2 TEMP=	195.0	DEG F	DEV= 0.2886
PLATE 3 TEMP=	179.4	DEG F	DEV= 0.1625
PLATE 4 TEMP=	171.6	DEG F	DEV= 0.1826
PLATE 5 TEMP=	162.8	DEG F	DEV= 0.2297
PLATE 6 TEMP=	155.9	DEG F	DEV= 0.1443
PLATE 7 TEMP=	151.4	DEG F	DEV= 0.1420
PLATE 8 TEMP=	148.2	DEG F	DEV= 0.0459
COND TEMP =	144.0	DEG F	DEV= 0.1118
STEAM TEMP =	233.1	DEG F	DEV= 0.2175
COND'T TEMP =	230.0	DEG F	DEV= 0.0914
REFLUX FLOW =	125.3	DEG F	DEV= 0.1344
FEED FLOW =	88.0	DEG F	DEV= 0.1291
BOTTOM FLOW =	102.1	DEG F	DEV= 0.1381
REB O'HEAD =	207.7	DEG F	DEV= 0.1900
FEED INLET =	163.5	DEG F	DEV= 0.1787
REFLUX INLET=	150.6	DEG F	DEV= 0.2500
COL O'HEAD =	148.6	DEG F	DEV= 0.1395
WATER INLET =	60.0	DEG F	DEV= 0.0757
WATER OUTLET=	85.2	DEG F	DEV= 0.1344

MAINLINE ONOFF

```
MAINLINE ONOFF
C
C
C        ***********************************
C        *                                 *
C        *         PROGRAM  ONOFF          *
C        *         --------------          *
C        *                                 *
C        ***********************************
C
C
C     PURPOSE
C        PERFORM CERTAIN USEFUL FUNCTIONS SUCH AS
C             TURN SPECIFIED LOOP RECORDS ON
C             (OPTION 1)
C             TURN SPECIFIED LOOP RECORDS OFF
C             (OPTION 2)
C             TURN SPECIFIED RING BUFFER LOOPS ON
C             (OPTION 3)
C             TURN SPECIFIED RING BUFFER LOOPS OFF
C             (OPTION 4)
C             INITIATE BUFFERING TO DISK
C             (OPTION 5)
C             INITIATE GAS CHROMATOGRAPH
C             (OPTION 8)
C             STOP GAS CHROMATOGRAPH
C             (OPTION 9)
C             CALL EXIT
C             (OPTION 6,7 OR 10)
C
C     USAGE
C        QUEUE FROM TELETYPE 9 AND ENTER DATA AS REQUIRED
C
C     REMARKS
C        ONOFF IS A PROCESS PROGRAM OPERATED IN AREA 4 UNDER
C        MPX
C        LOOPS 153,154 ARE R.B.T. LOOPS OF THE EVAPORATOR
C
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C        CHRTM
C        THIS SUBROUTINE SHOULD BE STORED IN THE COMPUTER
C        BEFORE LOADING THE MAINLINE PROGRAM
C
C     D.D.C. LOOP RECORDS REQUIRED
C        170,171,172,173,174,175,176,178,180,181,182,183,184
C        ,185,186, 187,188,153,154,210,211,212,213,214,215,
C        216,221,222,223,224, 225,226,227,228,201,202
C
```

MAINLINE ONOFF ...(CONT'D)

```
      EXTERNAL CHRTM
      DEFINE FILE 1(60,80,U,IRC)
      DEFINE FILE 2(100,16,U,KNEXT)
      DIMENSION ZERO(8),LPID(19),LPBF(17)
      DATA NLOOP/17/
      DATA NBUFF/15/
      DATA LPID/170,171,172,173,174,175,176,178,180,181,182
     *,183,184,
     1185,186,187,188,153,154/
      DATA LPBF/210,211,212,213,214,215,216,221,222,223,224
     *,225,226,
     1227,228/
      DATA ZERO/8*0./
      DATA NO/0/
      DATA LPHX/Z154/

C         DETERMINE WHICH TELETYPE TO USE
C

      IIN  = 9
      IOUT = IIN

C         ENTER WHICH OPTION TO USE
C         OPTION
C         1 TO MAKE LOOPS OPERABLE
C         2 TO MAKE LOOPS NONOPERABLE
C         3 TO MAKE RING BUFFERS  OPERABLE
C         4 TO MAKE RING BUFFERS NONOPERABLE
C         5 TO START BUFFERING TO DISK
C         6 CALL EXIT
C         7 CALL EXIT
C         8 TO START G. C.
C         9 TO STOP G. C.
C

1     WRITE(IOUT,2)
2     FORMAT(1H0,'ENTER OPTION')
10    CALL FFINP(IIN,1,0,IOPT,IERR)
      IF(IERR) 10,20,20
20    GO TO (50,100,150,200,250,1000,1000,400,450,1000,1000
     *,1000),IOPT

C     OPTION 1 MAKE DATA ACQUISTION LOOPS OPERABLE

   50 CONTINUE
      DO 60  I=1,NLOOP
60    CALL OPER(LPID(I))
      WRITE(IOUT,51)
51    FORMAT('LOOPS ON')
```

MAINLINE ONOFF ...(CONT'D)

```
C     CHECK FOR EVAPORATOR RBT LOOP

      CALL FNDLP(LPHX,LPAD)
      IF(LPAD)70,70,1
   70 CONTINUE
      CALL OPER(LPID(NLOOP+1))
      CALL OPER(LPID(NLOOP+2))
      GO TO 1

C     OPTION 2  MAKE DATA ACQUISTION LOOPS NONOPERABLE

  100 CONTINUE
      DO 110  I=1,NLOOP
110   CALL NONOP(LPID(I))
      WRITE(IOUT,101)
101   FORMAT('LOOPS OFF')
      GO TO 1

C     OPTION 3 MAKE RING BUFFERS OPERABLE

  150 DO 160  I=1,NBUFF
160   CALL OPER(LPBF(I))
      WRITE(IOUT,151)
151   FORMAT('RING BUFFERS ON')
      GO TO 1

C     OPTION 4   MAKE RING BUFFERS NONOPERABLE

  200 DO 210  I=1,NBUFF
210   CALL NONOP(LPBF(I))
      WRITE(IOUT,201)
201   FORMAT('RING BUFFERS OFF')
      GO TO 1

C     OPTION 5 START BUFFERING TO DISK

  250 DO 260 I=1,NBUFF
      CALL CVID(LPBF(I),LPHEX)
      CALL RSLP(LPHEX,LPAD)
260   CALL OPER(LPBF(I))
      WRITE(IOUT,251)
251   FORMAT(' BUFFERING TO DISK INITIALIZED')

C     WRITE TIME OF RUN INITIALIZATION ON GC PRINT OUT ON
C     TELETYPE NO. 1

      CALL TIME (IHR,IMIN,ISEC)
      WRITE (10,270) IHR,IMIN,ISEC
  270 FORMAT (T25, I3, '/', I3, '/', I3, T40, 'NEW RUN
     * INITIALIZED****')
```

MAINLINE ONOFF ...(CONT'D)

```
      WRITE (1'20) NO,IHR,IMIN,ISEC
      GO TO 1

C     OPTION 8   START GC
C        DETERMINE WHICH COMPOSITION TO MEASURE - FEED OR
C        BOTTOM
C        SUB OPTION 0 - MEASURE BOTTOM PRODUCT COMPOSITION
C        SUB OPTION 1 - MEASURE FEED COMPOSITION

400   WRITE(IOUT,402)
402   FORMAT('  ENTER 0 FOR NORMAL RUN 1 FOR FEED RUN')
405   CALL FFINP(IIN,1,0,IOPT,IERR)
      IF(IERR) 405,407,405
407   CONTINUE
      IF(IOPT) 430,430,431
430   WRITE (IOUT,433)
433   FORMAT (T5,'NORMAL RUN, IOPT = 0')
      GO TO 409
431   CONTINUE
      WRITE (IOUT,436)
436   FORMAT (T5,'FEED RUN, IOPT = 1')
409   CONTINUE
      CALL OPER(201)
      CALL OPER(202)
      ICYLE = 1500+200*IOPT
      CALL CYCLE(11,1,11,ICYLE)

C     SAMPLE INJECT

      CALL DOUT1(1,8,1)

C     LOOP FOR FIVE SECONDS

      CALL TIME(IHR,IMIN,ISEC)
410   CALL TIME(JHR,JMIN,JSEC)
      T=3600.*(JHR-IHR)+60.*(JMIN-IMIN)+JSEC-ISEC
      IF(T-5)410,410,420
420   CALL DOUT1(1,8,0)
      WRITE(IOUT,401)
401   FORMAT(' GC ON')
      WRITE (1'20) NO
      GO TO 1000

C     OPTION 9     STOP GC

450   CALL NONOP(202)
      CALL NONOP(201)
      CALL CANCL(11)
      WRITE(IOUT,451)
451   FORMAT('  GC OFF')
```

MAINLINE ONOFF ...(CONT'D)

```
1000  CALL EXIT
      END
```

SUBPROGRAM CHRTM

```
      SUBPROGRAM CHRTM
C
C
C                    SUBPROGRAM  CHRTM
C                    -----------------
C
C
C     PURPOSE
C        CONTROL THE GAS CHROMATOGRAPH
C
C     USAGE
C        THIS PROGRAM IS ACTIVATED BY ONOFF MAINLINE PROGRAM
C        WHEN BIT 1, LEVEL 11 IS ON (AREA 4)
C
C     SUBROUTINES OR SUBPROGRAMS REQUIRED
C        GC AND PEAK
C
C     REMARKS
C        CHRTM IS AN INTERRUPT CORELOAD
C        THE FOLLOWING DDC LOOPS ARE REQUIRED
C        201,202
C
C

      DEFINE FILE 1(100,16,U,KNEXT), 2(60,80,U,K2)
      DIMENSION COMP(5),RFCTR(5),IDATA(127),IERR(3),START(2)
     *,END(2)
      DIMENSION IHR1(80), IMIN1(80), ISEC1(80), ICOMP(80)
      DATA LPID,LPHEX/202,Z202/
      DATA RFCTR/5*1./
      DATA START/0.,30./
      DATA END/30.,110./

C     G.C. RESULTS ARE PRINTED OUT ON TELETYPE 10

      DATA IOUT/10/
      DATA IMASK/Z00FF/
      DATA NO/120/

C     STOP DATA ACQUISITION

      CALL NONOP(LPID)

C     SAMPLE INJECT
C     CLOSE ECO

      CALL DOUT1(1,8,1)

C     EXTRACT DATA FROM LOOP RECORD
```

SUBPROGRAM CHRTM ...(CONT'D)

```
C     GET ADDRESS OF LOOP RECORD

      CALL FNDLP(LPHEX,LPAD)

C     CHECK IF LOOP FOUND

      IF(LPAD)10,10,20
10    WRITE(IOUT,11)
11    FORMAT('  LOOP NOT FOUND  ')
      GO TO 250

C     GET CURRENT POSITION OF RING BUFFER POINTER

20    IPNTR=IAND(LD(LPAD+4),IMASK)

C     CHECK FOR ZERO POINTER IN RING BUFFER

      IF(IPNTR)21,21,25
21    IPNTR=7

C     TRANSFER DATA FROM RING BUFFER TO VECTOR IDATA

25    DO 60 I=1,120
      IF(IPNTR-126)40,40,30
30    IPNTR=7
40    IDATA(I)=LD(LPAD+IPNTR)
60    IPNTR=IPNTR+1

C     PROCESS DATA

      CALL GC(COMP,START,END,RFCTR,1.,IDATA,2,NO,IERR)

C     CHECK GC ERROR PARAMETERS

      DO 80 I=1,3
      IF(IERR(I))70,80,70
70    WRITE(IOUT,75)I,IERR(I)
80    CONTINUE
75    FORMAT('   ERROR NO ',I2,' = ',I5)
      CALL TIME(IHR,IMIN,ISEC)

C     CHECK WHICH CALIBRATION TO USE

      IF(COMP(2))130,130,120
120   IF(COMP(2)-.20)140,160,160

C     BOTTOM PRODUCT COMPOSITION

140   COMP(2)=105.92*COMP(2)+.224
130   CALL PTVLU(375,1,COMP(2),IER)
```

SUBPROGRAM CHRTM ...(CONT'D)

```
      GO TO 180

C     FEED COMPOSITION

160   COMP(2)=97.33*COMP(2)+1.934
180   WRITE(IOUT,181)IHR,IMIN,ISEC,COMP(2)
181   FORMAT(I10,'/',I2,'/',I2,'   G.C.  RESULTS --
     * COMPOSITION = '
     1,F10.3//)

C     OPEN ECO

      CALL DOUT1(1,8,0)

C     RESTART DATA ACQUISITION

      CALL OPER(LPID)

C     WRITE DATA TO FILE---TIME AND COMPOSITION

      READ (2'20) NDATA,IHRS,IMINS,ISECS
      WRITE (IOUT,9000) NDATA,IHRS,IMINS,ISECS
9000  FORMAT (T10, 'NDATA=', 4I5)
      IF (NDATA) 280,280,270
270   IF (NDATA-80) 275,250,250
275   READ (2'21) (IHR1(I), I=1,NDATA)
      READ (2'22) (IMIN1(I), I=1,NDATA)
      READ (2'23) (ISEC1(I), I=1,NDATA)
      READ (2'24) (ICOMP(I), I=1,NDATA)


280   NDATA=NDATA+1
      IHR1(NDATA)=IHR
      IMIN1(NDATA)=IMIN
      ISEC1(NDATA)=ISEC
      ICOMP(NDATA)=COMP(2)*100.
      WRITE (2'20) NDATA,IHRS,IMINS,ISECS
      WRITE (2'21) (IHR1(I), I=1,NDATA)
      WRITE (2'22) (IMIN1(I), I=1,NDATA)
      WRITE (2'23) (ISEC1(I), I=1,NDATA)
      WRITE (2'24) (ICOMP(I), I=1,NDATA)
250   CALL EXIT
      END
```

SUBROUTINE PEAK

```
      SUBROUTINE  PEAK(Y,NPTS,IER)
C
C
C                 SUBROUTINE  PEAK
C                 ----------------
C
C
C     PURPOSE
C        1. DETERMINE THE START OF A PEAK (ISTRT) AND THE
C        END OF A PEAK (IEND) BY EXAMINATION OF FIRST
C        DERIVATIVES
C        2. DETERMINE IF THE BASE LINE IS REACHED AT THE END
C        OF A PEAK, IF YES, SET NBASE EQUAL TO 1
C        3. CHECK THE DATA FOR ANY VALUE LESS THAN 0 OR
C        EQUAL TO 32767
C
C     DESCRIPTION OF PARAMETERS
C        Y         VECTOR OF INPUT DATA INTEGERS
C        NPTS      NUMBER OF DATA POINTS
C        IER       ERROR CODES
C        IER(1)    = 0 ... O. K.
C        IER(1)    +VE ... END OF DATA DURING PEAK ELUTION
C                  THEN IER(1) IS EQUAL TO THE VALUE OF
C                  THE DERIVATIVE AT PEAK END
C        IER(2)    NUMBER OF BAD DATA POINTS (I.E. POINTS OF
C                  LESS THAN 0 OR EQUAL TO 32767)
C        IER(3)    = 0 ... O. K.
C        IER(3)    = 1 ... NUMBER OF PEAKS FOUND IS DIFFE-
C                  RENT FROM NUMBER OF PEAKS SPECIFIED
C
C     USAGE
C        CALL PEAK(Y,NPTS,IER)
C
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C        NONE
C
C

      INTEGER Y(1)
      DIMENSION IER(3)
      COMMON H,ISTRT(5),IEND(5),NBASE(5),NPEAK
      DATA DBST,DBEND,DB2,ITEST/3.,5.,3.,3/
      DATA DRV1,DRV1A,ICFST,ICFED,NCOND,NGHG/0.,0.,0,0,0,0/
      NDATA=NPTS-4
      DO 200 I=3,NDATA

C     DATA INTEGERTY CHECK

      IF(Y(I))6,7,7
```

SUBROUTINE PEAK ...(CONT'D)

```
6       IER(2)=IER(2)+1
        GO TO 9
7       IF(Y(I)-32767)9,8,8
8       IER(2)=IER(2)+1

C       COMPUTE FIRST DERIVATIVE AT Y(I-1)

9       DRV1B=DRV1

C       COMPUTE FIRST DERIVATIVE AT Y(I)

        DRV1=DRV1A

C       COMPUTE FIRST DERIVATIVE AT Y(I+1)
C       SEVEN POINT LEAST SQUARES ESTIMATE OF FIRST DERIVATIVE

        DRV1A=3.*(Y(I+4)-Y(I-2))+2.*(Y(I+3)-Y(I-1))+
       1Y(I+2)-Y(I)
        DRV1A=DRV1A/(28.*H)

C       IS PEAK IN PROGRESS

        IF(NCOND)10,10,40

C       PEAK IS NOT IN PROGRESS
C       CHECK FIRST DERIVATIVE FOR PEAK START

10      IF(DRV1-DBST)190,20,20

C       CONFIRM PEAK START ITEST TIMES

20      ICFST=ICFST+1
25      IF(ICFST-ITEST)200,30,30

C       PEAK HAS STARTED

30      NCOND=1

C       INCREMENT PEAK COUNTER

        NPEAK=NPEAK+1
        NBASE(NPEAK)=0

C       SAVE INDEX OF STARTING POINT

        ISTRT(NPEAK)=I-ITEST+1
        ICFST=0
        GO TO 200

C       CHECK FOR PEAK END
```

SUBROUTINE PEAK ...(CONT'D)

```
C       HAS FIRST DERIVATIVE GONE +VE TO -VE

40      IF(NGHG)50,50,70
50      IF(DRV1)60,200,200

C       FIRST DERIVATIVE HAS GONE +VE TO -VE

60      NGHG=1

C       CHECK FOR PEAK END

70      IF(DRV1+DBEND)190,80,80

C       CONFIRM PEAK END

80      ICFED=ICFED+1

C       CHECK FOR START OF NEW PEAK

        IF(DRV1-DBST)77,75,75
75      ICFST=ICFST+1
        GO TO 78
77      ICFST=0
78      IF(ICFED-ITEST)200,87,87

C       PEAK END
C       SAVE INDEX OF END POINT

87      IEND(NPEAK)=I-ITEST+1

C       COMPUTE 2ND DEIVATIVE AT PEAK END

        DRV2=(DRV1A-DRV1B)/(2.*H)

C       REST INDICATORS

        ICFED=0
        NCOND=0
        NGHG=0

C       CHECK FOR IMMEDIATE START OF NEW PEAK

        IF(ICFST)88,88,25

C       CHECK IF BACK ON BASE LINE AT PEAK END

88      IF(DRV2-DB2)90,90,200

C       BACK ON BASE LINE
```

SUBROUTINE PEAK ...(CONT'D)

```
90     NBASE(NPEAK)=1
190    ICFED=0
       ICFST=0
200    CONTINUE

C      END OF DATA SET
C      CHECK FOR ERROR

       IF(NPEAK)250,250,205
205    IF(NCOND)250,250,210

C      END OF DATA DURING PEAK ELUTION

210    IER(1)=DRV1
       IEND(NPEAK)=NPTS-2
       NBASE(NPEAK)=1
250    RETURN
       END
```

SUBROUTINE GC

```
      SUBROUTINE  GC  (AREA,START,END,RFCTR,PTSEC,Y,NUMBR
     *,NPTS,IER)
C
C
C                 SUBROUTINE  GC
C                 --------------
C
C
C     PURPOSE
C        COMPUTE AREAS FOR DIFFERENT PEAKS FOUND BY
C        SUBROUTINE PEAK
C
C     DESCRIPTION OF PARAMETERS
C        AREA      CALCULATED COMPOSITIONS
C        START     START OF TIME BAND FOR PEAK
C        END       END OF TIME BAND FOR PEAK
C        RFCTR     VECTOR OF RESPONSE FACTORS
C        PTSEC     POINTS PER SECOND
C        Y         VECTOR OF INPUT DATA INTEGERS
C        NUMBR     NUMBER OF PEAKS EXPECTED
C        NPTS      NUMBER OF DATA POINTS
C        IER       ERROR CODES (DEFINED IN SUBROUTINE PEAK)
C
C     USAGE
C        CALL GC(AREA,START,END,RFCTR,PTSEC,Y,NUMBR,NPTS
C        ,IER)
C
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C        NONE
C
C
      INTEGER Y(1)
      DIMENSION AREA(1),START(1),END(1),RFCTR(1),IER(3)
      COMMON H,ISTRT(5),IEND(5),NBASE(5),NPEAK
      START(1)=0.
      NPEAK=0
      NO=1
      DO 5 I=1,3
5     IER(I)=0
      H=1./PTSEC
C     CALL SUBROUTINE PEAK   FIND START AND END OF ALL PEAKS
      CALL PEAK(Y,NPTS,IER)
      IF(NPEAK)250,250,7
7     CONTINUE
C     CALCULATE SIMPSONS RULE AREAS FOR PEAKS DETECTED
```

SUBROUTINE GC ...(CONT'D)

```
      DO 120 K=1,NPEAK
      AREA(K)=0.
C     CHECK IF NUMBER INTERVALS EVEN OR ODD
      L=IEND(K)-ISTRT(K)
      X=FLOAT(L)/2.
      L=L/2
      IF(X-L)20,20,10
C     ODD NUMBER OF INTERVALS   ADD ONE INTERVAL TO PEAK
10    IEND(K)=IEND(K)+1
20    IBGN=ISTRT(K)+1
      JEND=IEND(K)-1
C     SIMPSONS RULE INTEGRATION
      DO 40 I=IBGN,JEND,2
40    AREA(K)=AREA(K)+4.*Y(I)+2.*Y(I+1)
      AREA(K)=AREA(K)+Y(IBGN-1)-Y(JEND+1)
      AREA(K)=AREA(K)/3.
C     CHECK IF BACK ON BASE LINE
      IF(NBASE(K))115,115,50
C     BACK ON BASE LINE
C     FIT LEAST SQUARES LINE TO DATA IMMEDIATELY BEFORE AND
C     AFTER PEAK
50    SMXY=0.
      SMY=0.
      SMX=0.
      SMX2=0.
      L=0
      IBGN=ISTRT(NO)-3
      JEND=IEND(K)-1
C     FOR DATA BEFORE LAST PEAK ON BASE LINE
      DO 60 I=1,2
      L=L+1
      X=IBGN+I
      II=IBGN+I
      SMXY=SMXY+Y(II)*X
      SMY=SMY+Y(II)
      SMX=SMX+X
60    SMX2=SMX2+X**2
```

SUBROUTINE GC ...(CONT'D)

```
C     FOR DATA AFTER PRESENT PEAK

      DO 90 J=1,2
      X=JEND+J
      II=JEND+J
      L=L+1
      SMXY=Y(II)*X+SMXY
      SMY=SMY+Y(II)
      SMX=SMX+X
      SMX2=SMX2+X**2
90    CONTINUE
      X=L

C     EQUATION OF LEAST SQUARES LINE  Y=SLOPE*X+A
C
C     COMPUTE SLOPE OF LEAST SQUARES LINE

      SLOPE=(SMXY-SMX*SMY/X)/(SMX2-SMX**2/X)

C     COMPUTE INTERCEPT OF LEAST SQUARES LINE

      A=SMY/X-SLOPE*SMX/X

C     CORRECT AREAS

      DO 110 I=NO,K
      C=A+SLOPE/2.*(ISTRT(I)+IEND(I))
110   AREA(I)=AREA(I)-C*(IEND(I)-ISTRT(I))
      NO=K+1
      GO TO 120
115   CONTINUE
120   CONTINUE

C     CHECK IF NO. PEAKS FOUND = NO. SPECIFIED

      IF(NUMBR-NPEAK)122,125,122
122   IER(3)=1
125   X=0.

C     ASSIGN  AREAS TO APPROPRIATE TIME BANDS
C     TIME BANDS SPECIFIED RELATIVE TO START OF FIRST PEAK
C     REFERENCE TIME = START OF FIRST PEAK

      REFTM=ISTRT(1)*H
      DO 220 I=1,NUMBR
      BAND=0.
      DO 200 J=1,NPEAK
      TSTRT=H*ISTRT(J)

C     IS PEAK START IN THIS TIME BAND
```

SUBROUTINE GC ...(CONT'D)

```
      IF(START(I)+REFTM-TSTRT)160,160,200
160   IF(END(I)+REFTM-TSTRT)200,200,180

C     ADD PEAK AREAS IN THIS TIME BAND

180   BAND=BAND+AREA(J)
200   CONTINUE
220   AREA(I)=BAND

C     CALCULATE COMPOSITIONS

      DO 130 I=1,NUMBR
130   X=X+AREA(I)*RFCTR(I)
      DO 140 I=1,NUMBR
140   AREA(I)=AREA(I)*RFCTR(I)/X
250   RETURN
      END
```

MAINLINE GTDAT

```
      MAINLINE GTDAT

C
C
C         ***********************************
C         *                                 *
C         *         PROGRAM  GTDAT          *
C         *         --------------          *
C         *                                 *
C         ***********************************
C
C
C     PURPOSE
C        EXTRACT DATA BUFFERED TO DISK FROM DDC AND CONVERT
C        TO ENGINEERING UNITS
C        OUTPUT DATA ARE PUNCHED ONTO CARDS IN 10F8.3 FORMAT
C
C     DESCRIPTION OF PARAMETERS
C        NLOOP     NUMBER OF RING BUFFERS
C        NPTS      NUMBER OF DATA POINTS TO BE SORTED
C        IDELT     POLL TIME FOR RING BUFFERS (SEC.)
C        IGC       PROGRAM CONTROL FLAG
C                  ... 1 DUMP G.C. DATA FROM FILES
C                  ...-1 DO NOT DUMP G.C. DATA FROM FILES
C        TITLE     RUN TITLES
C        LPID      LOOP ID'S OF RING BUFFERS
C        A         CONA OF THE CORRESPONDING DDC LOOP
C        B         CONB OF THE CORRESPONDING DDC LOOP
C        TEMPT     TEMPERATURE OF THE CORRESPONDING DDC LOOP
C                  (USED FOR FLOW CORRECTION)
C                  ...-1 FLOW CORRECTION IS NOT NECESSARY
C        CMPSN     COMPOSITION (WT P C) OF THE FLOW LOOP
C        NAME1,2   TITLES OF THE CORRESPONDING RING BUFFERS
C        FILE 1    NIGBD USER INTERFACE
C        FILE 2    OUTPUT FILE
C        FILE 3    DAFLE
C        FILE 5    G.C. FILE
C
C     USAGE
C        ENTER DATA CARDS AS REQUIRED
C
C     REMARKS
C        THIS IS A NONPROCESS PROGRAM WHICH IS ABLE TO SORT
C        DATA UP TO 10 LOOP RECORDS. THE FOLLOWING FILES ARE
C        NECESSARY
C        FILE 3    DAFLE (PROVIDED BY DACS CENTRE)
C        FILE 5    PAC01
C
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C        NIGBD, GBOUT, GBSRT (PROVIDED BY DACS CENTRE)
```

MAINLINE GTDAT ...(CONT'D)

```
C
C
      DEFINE FILE 1(8,80,U,K),2(50,80,U,K),3(64,320,U,K),4(8
     *,160,U,K)
      DEFINE FILE 5(60,80,U,K5)
      REAL NAME1(20),NAME2(20)
      INTEGER DAOUT(320)
      DIMENSION X(10,80),A(10),B(10),LPID(10),TEMPT(10),
     1CMPSN(10),TITLE(20)
      DIMENSION LIME(3)
      DIMENSION IHR(80), IMIN(80), ISEC(80),ICOMP(80)
      DATA NO/80/
C         DEFINE FLOW CONVERSION FUNCTIONS
      TEMP(T)=5.*(T-32.)/9.
      DENS(T,X)=1.0201-0.5123E-03*T-0.1512E-05*T**2-0.1519E
     *-02*100.*X
     1    -0.8106E-05*(100.*X)**2
C         READ INPUT DATA
      READ (5,1) NLOOP,NPTS,IDELT , IGC
    1 FORMAT (4I5)
      READ(5,3)(TITLE(I),I=1,20)
    3 FORMAT(20A4)
      WRITE(6,2)NLOOP,NPTS
    2 FORMAT(' ',20X,'NUMBER OF LOOPS',I5/21X,'NUMBER DATA
     * PTS',I5)
      K=-1
      DO 10 I=1,NLOOP
      K=K+2
      J=K+1
   10 READ (5,4) LPID(I),A(I),B(I),TEMPT(I),CMPSN(I)
     *,(NAME1(N),N=K,J),
     1(NAME2(N),N=K,J)
    4 FORMAT (I10,4F10.2,4A4)
      WRITE(6,5)
    5 FORMAT(' ',////,20X,'LOOP NO.',10X,'CONSTANT A',10X
     *,'CONSTANT B',
     1)
      WRITE(6,6)(LPID(I),A(I),B(I),I=1,NLOOP)
    6 FORMAT(' ',20X,I5,10X,F10.4,10X,F10.5)
      READ(5,7)
    7 FORMAT(72X)
      IF (IGC) 9,8,8
C         IGC   +VE ... DUMP G.C. DATA FROM FILES
```

MAINLINE GTDAT ...(CONT'D)

```
    8 READ (5'20) NDATA, IHRS, IMINS, ISECS
      READ (5'21) (IHR(I), I=1,NDATA)
      READ (5'22) (IMIN(I), I=1,NDATA)
      READ (5'23) (ISEC(I), I=1,NDATA)
      READ (5'24) (ICOMP(I), I=1,NDATA)

C         WRITE OUT G.C. DATA

      WRITE(6,9000) NDATA
 9000 FORMAT (T40, 'NDATA=', I5)
      WRITE (6,12) IHRS,IMINS,ISECS
   12 FORMAT ('1'//// T48, 'GC RESULTS'//T40, I5, '/', I5, '
     */', I5,
     ' '   STARTING TIME'//T47, 'TIME', T60, 'COMP'/ )
      DO 11 I=1,NDATA
      COMP=ICOMP(I)/100.
      WRITE (6,15) IHR(I), IMIN(I), ISEC(I), COMP
   15 FORMAT (T40,I5,'/',I5,'/',I5,F10.3)
   11 CONTINUE
      WRITE (5,16) IHRS,IMINS,ISECS
   16 FORMAT (3I5, 25X, 'STARTING TIME')
      DO 14 I=1,NDATA
      COMP=ICOMP(I)/100.
      WRITE (5,13) IHR(I),IMIN(I),ISEC(I),COMP
   13 FORMAT (3I5, F10.3)
   14 CONTINUE
      WRITE (6,17)
   17 FORMAT ('1')

C         DEFINE PARAMETERS FOR NIGBD

    9 CONTINUE
      IKIN = 3
      IKOUT = 1
      JRECW = 80
      JRECR = 8
      IF(NPTS-80)20,20,40
   20 NO=NPTS
   40 NREC=NPTS/80
      IF(NPTS-NREC*80)250,80,60
   60 NREC=NREC+1
   80 KRCNO=0

C         CONVERT LOOP ID'S TO HEXADECIMAL

      DO 160 I=1,NLOOP
      CALL CVID(LPID(I),IFUNC)

C         SORT NIGBD FOR THE SPECIFIED LOOP RECORD
```

MAINLINE GTDAT ...(CONT'D)

```
      CALL NIGBD(IFUNC,NPTS,JRECW,JRECR,IKIN,IKOUT,LIME
     *,IERR1,IERR2)
C         CHECK NIGBD ERROR PARAMETER
      IF(IERR1-1) 100,448,100
  100 WRITE(6,101) LPID(I),IERR1
  101 FORMAT(' ',10X,'LOOP ID',I10/11X,'NIGBD ERROR',I10)
      NPTS = IERR2
  448 CONTINUE
      WRITE (6,777) LIME(1),LIME(2),LIME(3)
  777 FORMAT (10X,'TIME LAST VALUE WAS BUFFERED IN DISK IS
     * =',I5,'.',I5,
     1'.',I5///)
C         TRANSFER DATA FROM INTERFACE FILE TO OUTPUT FILE
      DO 160 IRCNO=1,NREC
      READ(1'IRCNO) DAOUT
      KRCNO=KRCNO+1
      WRITE(2'KRCNO) DAOUT
      IF(KRCNO-50)160,160,250
  160 CONTINUE
C         ALL DATA ARE IN OUTPUT FILE
      WRITE(6,161)(TITLE(I),I=1,20),NPTS,IDELT
      WRITE(6,162)(NAME1(I),I=1,20)
      WRITE(6,162)(NAME2(I),I=1,20)
      WRITE(6,165)
      WRITE(5,163)(TITLE(I),I=1,20),NPTS,IDELT
      WRITE(5,166)(NAME1(I),I=1,20)
      WRITE(5,166)(NAME2(I),I=1,20)
  161 FORMAT('1',20X,20A4,///35X,'NO. DATA POINTS',I5,'
     * TIME INCREMENT
     1'I5,'  SEC.'///)
  162 FORMAT(' ',10X,10(2X,2A4))
  163 FORMAT(20A4,/10X,'NO. POINTS',I5,'  DELT T',I5,'
     * SEC.')
  165 FORMAT(' ',///)
  166 FORMAT(20A4)
      DO 220 N=1,NREC
      KRCNO=N
      DO 200 I=1,NLOOP
      READ(2'KRCNO) DAOUT
      KRCNO=KRCNO+NREC
C         CONVERT TO ENGINEERING UNITS
      DO 180 K=1,80
```

MAINLINE GTDAT ...(CONT'D)

```
  180 X(I,K) = A(I)/32767.0*DAOUT(K)+B(I)
C         CHECK FOR FLOW CORRECTION
      IF (TEMPT(I)) 200,200,190
C         CORRECT FLOWS
  190 CORRT=SQRT(DENS(TEMP(TEMPT(I)),CMPSN(I)/100.))
      DO 195 J=1,80
      X(I,J)=X(I,J)*CORRT
  195 CONTINUE
  200 CONTINUE
C         PRINT OUT AND PUNCH ALL THE DATA
      DO 205 J=1,NO
  205 WRITE(6,206)(X(I,J),I=1,NLOOP)
      DO 207 J=1,NO
  207 WRITE(5,208)(X(I,J),I=1,NLOOP)
  206 FORMAT(' ',10X,10F10.3)
  208 FORMAT(10F8.3)
C         CHECK IF ALL DATA WERE SORTED OUT
      IF(NPTS-N*80-79)210,210,220
  210 NO=NPTS-N*80
  220 CONTINUE
  250 WRITE (6,260)
  260 FORMAT ('1')
      CALL EXIT
      END
```

APPENDIX E

DETERMINATION OF THE CONTROL TRAY BY THE ROSENBROCK METHOD

To determine the "optimum" control tray by Rosenbrock's method, if reflux flow is used as the manipulative variable, the strategy is to prevent any change in composition on one of two trays where the desired liquid composition is:

$$x_i = x_f \pm \frac{1}{4}(x_D - x_W) \quad . \tag{E.1}$$

If steam flow is to be manipulated, the strategy is to maintain the composition on the tray where the desired vapor composition is:

$$y_i = y_f \pm \frac{1}{4}(x_D - x_W) \quad . \tag{E.2}$$

E.1 Location of the "Optimum" Control Tray for the University of Delaware Column

For the University of Delaware column, the following data were given for the test designated as Run No. 8 by Gerster et al.

x_f = 43.2 mole % acetone	y_f = 54.7 mole % acetone
x_D = 79.2 mole % acetone	x_W = 8.1 mole % acetone
x_9 = 61.8 mole % acetone	y_9 = 74.1 mole % acetone
x_1 = 11.4 mole % acetone	y_3 = 44.6 mole % acetone

Using these data, it is apparent that if reflux flow is used as the manipulative variable, either tray 9 or tray 1 should be used as the control tray and if steam flow is used as the manipulative variable, tray 9 or tray 3 should be used as the control tray.

E.2 Location of the "Optimum" Control Tray for the University of Alberta Column

For the University of Alberta column, the following data were obtained experimentally:

x_f = 38.0 weight % methanol y_f = 64.0 weight % methanol

x_D = 95.9 weight % methanol x_W = 0.6 weight % methanol

x_6 = 61.0 weight % methanol y_6 = 94.0 weight % methanol

x_2 = 10.0 weight % methanol y_2 = 40.0 weight % methanol

Calculations using these data using equations (E.1) and (E.2) reveals that by manipulation of reflux or steam flow, tray 6 or tray 2 should be used as the control tray.

In general, of top product composition is to be controlled, the sensor should be located in the rectifying section and if bottom product composition is to be controlled, the sensor should be located in the stripping section.